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* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  SEP 09   CA/CAplus records now contain indexing from 1907 to the
                   present
 NEWS  4  Jul 15   Data from 1960-1976 added to RDISCLOSURE
 NEWS  5  Jul 21   Identification of STN records implemented
 NEWS  6  Jul 21   Polymer class term count added to REGISTRY
 NEWS  7  Jul 22   INPADOC: Basic index (/BI) enhanced; Simultaneous Left and
                   Right Truncation available
 NEWS  8  AUG 05   New pricing for EUROPATFULL and PCTFULL effective
                   August 1, 2003
 NEWS  9  AUG 13   Field Availability (/FA) field enhanced in BEILSTEIN
 NEWS 10  AUG 15   PATDPAFULL: one FREE connect hour, per account, in
                   September 2003
 NEWS 11  AUG 15   PCTGEN: one FREE connect hour, per account, in
                   September 2003
 NEWS 12  AUG 15   RDISCLOSURE: one FREE connect hour, per account, in
                   September 2003
 NEWS 13  AUG 15   TEMA: one FREE connect hour, per account, in
                   September 2003
 NEWS 14  AUG 18   Data available for download as a PDF in RDISCLOSURE
 NEWS 15  AUG 18   Simultaneous left and right truncation added to PASCAL
 NEWS 16  AUG 18   FROSTI and KOSMET enhanced with Simultaneous Left and Righ
                   Truncation
 NEWS 17  AUG 18   Simultaneous left and right truncation added to ANABSTR
 NEWS 18  SEP 22   DIPPR file reloaded
 NEWS 19  SEP 25   INPADOC: Legal Status data to be reloaded
 NEWS 20  SEP 29   DISSABS now available on STN

 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 04:41:27 ON 01 OCT 2003

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    0.21       0.21

FILE 'REGISTRY' ENTERED AT 04:41:32 ON 01 OCT 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
```

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2
DICTIONARY FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

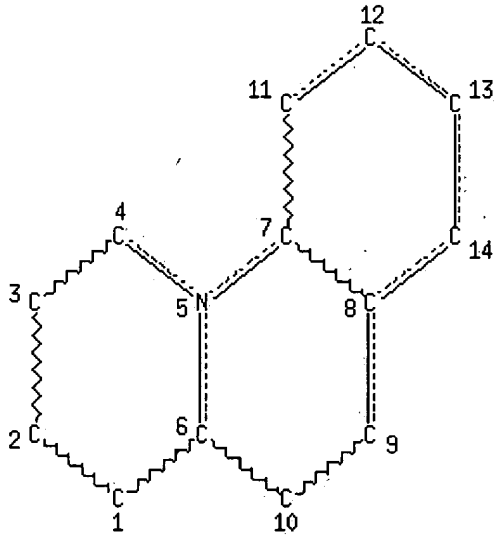
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
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NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS R AT 10
NSPEC IS R AT 11
NSPEC IS R AT 12
NSPEC IS R AT 13
NSPEC IS R AT 14

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE


=> s l1
SAMPLE SEARCH INITIATED 04:42:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1632 TO ITERATE

 61.3% PROCESSED    1000 ITERATIONS                              23 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       30217 TO    35063
PROJECTED ANSWERS:            383 TO     1117

L2            23 SEA SSS SAM L1

=>
L3       STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3               STR

=> s l3
SAMPLE SEARCH INITIATED 04:45:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    600 TO ITERATE

100.0% PROCESSED     600 ITERATIONS                               8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       10531 TO    13469
PROJECTED ANSWERS:              8 TO      329

L4             8 SEA SSS SAM L3

=> s l3 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 04:45:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  12373 TO ITERATE

100.0% PROCESSED   12373 ITERATIONS                            164 ANSWERS
SEARCH TIME: 00.00.01

L5           164 SEA SSS FUL L3

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
```

FULL ESTIMATED COST 150.55 150.76

FILE 'HCAPLUS' ENTERED AT 04:45:27 ON 01 OCT 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 1 Oct 2003 VOL 139 ISS 14
FILE LAST UPDATED: 30 Sep 2003 (20030930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

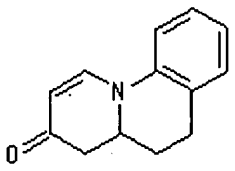
=> **s l5**
L6 42 L5

=> s l5 and pd < january 1998
42 L5
18793762 PD < JANUARY 1998
(PD<19980100)
L7 33 L5 AND PD < JANUARY 1998

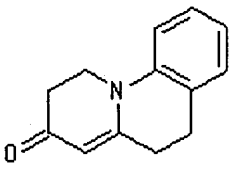
=> **d l7, ibib abs fhitstr, 1-33**

L7 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN
Full Text Citing References

ACCESSION NUMBER: 1998:713257 HCAPLUS
DOCUMENT NUMBER: 130:52313
TITLE: Synthesis of benzo[c]quinolizin-3-ones: selective non-steroidal inhibitors of steroid 5α-reductase 1
AUTHOR(S): Guarna, Antonio; Occhiato, Ernesto G.; Scarpi, Dina; Tsai, Ruey; Danza, Giovanna; Comerci, Alessandra; Mancina, Rosa; Serio, Mario
CORPORATE SOURCE: Dipartimento di Chimica Organica "U. Schiff", Centro di Studio sulla Chimica e la Struttura dei Composti Eterociclici e lori Applicazioni, CNR, Univ. di Firenze, Florence, I-50121, Italy
SOURCE: Bioorganic & Medicinal Chemistry Letters (**1998**), 8(20), 2871-2876
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



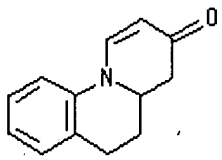
II

AB A short and efficient synthesis of novel benzo[c]quinolizin-3-ones I and II is described. The synthesis is based on the tandem Mannich-Michael cyclization between 2-(silyloxy)-1,3-butadienes and a N-t-Boc iminium ion. I and II are selective inhibitors of human steroid 5α-reductase isoenzyme 1, and thus have potential application as drugs for treatment of male pattern baldness and other DHT-dependent skin disorders.

IT **194979-80-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(benzo[c]quinolizin-3-ones as selective inhibitors of steroid 5α-reductase 1)

RN 194979-80-1 HCAPLUS

CN 3H-Benzo[c]quinolizin-3-one, 4,4a,5,6-tetrahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

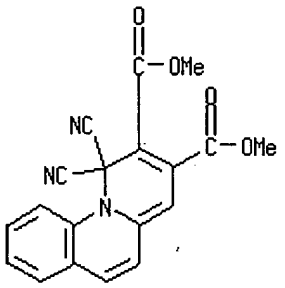
L7 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:289938 HCAPLUS
DOCUMENT NUMBER: 128:294736
TITLE: The reaction between triazolobenzopyridinium and triazolothiazolium ylides with dimethyl acetylenedicarboxylate
AUTHOR(S): Abarca, Belen; Ballesteros, Rafael; Houari, Nadia; Samadi, Aldelouahid
CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Farmacia, Universidad de Valencia, Valencia, 46100, Spain
SOURCE: Tetrahedron (**1998**), 54(15), 3913-3918
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reaction of some [1,2,3]triazolo[1,5-a]quinolinium, [1,2,3]triazolo[5,1-a]isoquinolinium, and [1,2,3]triazolo[5,1-b]thiazolium ylides with di-Me acetylenedicarboxylate is described. Compds. such as di-Me pyrrolo[1,2-a]quinoline-1,2-dicarboxylate, di-Me pyrrolo[2,1-a]isoquinoline-2,3-dicarboxylate, 1,1-dicyano-2,3-dimethoxycarbonyl-1H-pyrido[1,2-a]quinoline, 4,4-dicyano-2,3-dimethoxycarbonyl-4H-pyrido[2,1-a]isoquinoline, and 7-methyl-5,6-dimethoxycarbonylpyrrolo[2,1-a]thiazole, are formed.

IT 206189-66-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of triazolobenzopyridinium and triazolothiazolium ylides with di-Me acetylenedicarboxylate)
RN 206189-66-4 HCAPLUS
CN 1H-Benzo[c]quinolizine-2,3-dicarboxylic acid, 1,1-dicyano-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:542448 HCAPLUS
DOCUMENT NUMBER: 127:220585
TITLE: Benzo[c]quinolizine derivatives, their preparation and use as 5α-reductases inhibitors
INVENTOR(S): Guarna, Antonio; Serio, Mario
PATENT ASSIGNEE(S): Applied Research Systems ARS Holding N.V., Neth. Antilles; Guarna, Antonio; Serio, Mario
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

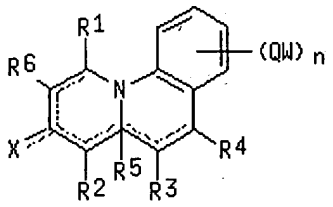
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9729107	A1	19970814	WO 1997-EP552	19970207 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9717672	A1	19970828	AU 1997-17672	19970207 <--
AU 711886	B2	19991021		
EP 880520	A1	19981202	EP 1997-903230	19970207
EP 880520	B1	20030416		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
EE 9800233	A	19981215	EE 1998-233	19970207
EE 4058	B1	20030616		
CN 1210536	A	19990310	CN 1997-192097	19970207
CN 1116296	B	20030730		

JP 2000504680	T2	20000418	JP 1997-528158	19970207
AT 237614	E	20030515	AT 1997-903230	19970207
EP 926148	A1	19990630	EP 1997-122733	19971223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
NO 9803444	A	19980724	NO 1998-3444	19980724
US 6303622	B1	20011016	US 1998-117583	19980729
CA 2315055	AA	19990708	CA 1998-2315055	19981221
WO 9933828	A1	19990708	WO 1998-EP8582	19981221
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9924194	A1	19990719	AU 1999-24194	19981221
AU 744105	B2	20020214		
BR 9813836	A	20001010	BR 1998-13836	19981221
EP 1066284	A1	20010110	EP 1998-966711	19981221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
EE 200000387	A	20011217	EE 2000-2000038719981221	
JP 2001527074	T2	20011225	JP 2000-526509	19981221
ZA 9811762	A	19990623	ZA 1998-11762	19981222
NO 2000003199	A	20000823	NO 2000-3199	20000620
US 2001044542	A1	20011122	US 2001-888952	20010625
US 6555549	B2	20030429		
US 2001047098	A1	20011129	US 2001-891088	20010625
US 6552034	B2	20030422		

PRIORITY APPLN. INFO.:	IT 1996-FI19	A	19960209
	WO 1997-EP552	W	19970207
	EP 1997-122733	A	19971223
	US 1998-117583	A1	19980729
	WO 1998-EP8582	W	19981221

OTHER SOURCE(S): MARPAT 127:220585

GI



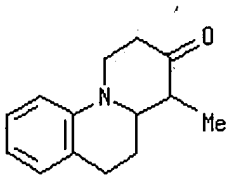
I

AB The benzo[c]quinolizine derivs. I (R1-R4, R6 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocycle, halo, amino azide, alkoxycarbonyl, etc.; R5 =H, alkyl, alkoxycarbonyl, cyano, aryl, heterocycle; X = O, acyl, alkoxycarbonyl, NO2, carbamoyl; Q = bond, alkyl, alkenyl, alkynyl, amino, etc., W = H, alkyl, alkenyl, alkynyl, aryl, aryloxy, amino, halo, etc.) were prepd. as 5α-reductases inhibitors (no data). Thus, N-(tert-butoxycarbonyl)-2-ethoxy-1,2,3,4-tetrahydroquinline was cyclized with 2-(trimethylsilyloxy)-1,3-butadiene to give 1,2,4,4a,5,6-hexahydro-(11H)-benzo[c]quinolizin-3-one.

IT **5569-24-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzo[c]quinolizine derivs. as 5α-reductases inhibitors)

RN 5569-24-4 HCAPLUS
CN 3H-Benzo[c]quinolizin-3-one, 1,2,4,4a,5,6-hexahydro-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1993:6845 HCAPLUS
DOCUMENT NUMBER: 118:6845
TITLE: Oxocarbons and related compounds. Part 18. The reaction of perchlorocyclobutenone with pyridines: a novel synthesis of 4H-4-quinolizinones
AUTHOR(S): Schmidt, Arthur H.; Duemmler, Mario
CORPORATE SOURCE: Abt. Org. Chem. Biochem., Fachlochsch. Fresenius, Wiesbaden, D-6200, Germany
SOURCE: Synthesis (**1992**), (10), 969-72
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 118:6845
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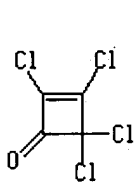

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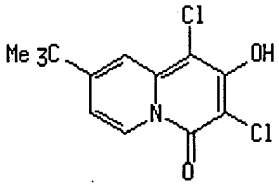
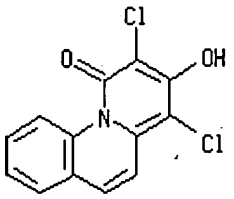


II

AB Heating of tetrachlorocyclobutenone (I) with pyridines followed by treatment with water affords 1,3-dichloro-2-hydroxy-4H-4-quinolizinones, e.g. II, and 1,3-dichloro-2-hydroxy-4-oxo-4H-quinolizinecarboxylates. The reaction did not proceed via intermediate (trichloropxocyclobutenyl)pyridinium salts to give betaines. The reaction pathway has been secured by trapping 1,2,3-trichloro-8-(1,1-dimethylethyl)-4H-4-quinoliznone and by its successive conversion to II on heating with water.

IT **144785-48-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by ring opening and reaction of perchlorocyclobutenone with pyridine)

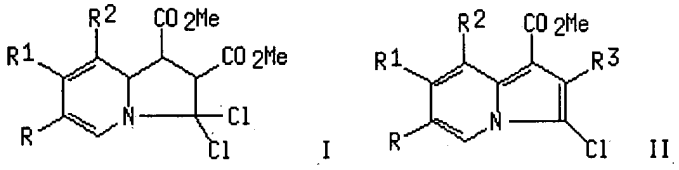
RN 144785-48-8 HCAPLUS
CN 1H-Benzo[c]quinolizin-1-one, 2,4-dichloro-3-hydroxy- (9CI) (CA INDEX NAME)



L7 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

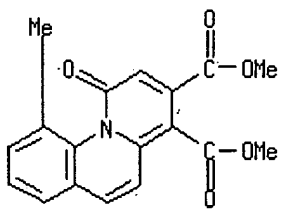
Full Text | Citing References

ACCESSION NUMBER: 1990:531933 HCAPLUS
DOCUMENT NUMBER: 113:131933
TITLE: 1,3-Dipolar cycloadditions of ylides formed from pyridine and dichlorocarbene
AUTHOR(S): Khlebnikov, A. F.; Kostik, E. I.; Kostikov, R. R.; Bespalov, V. Ya.
CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, 199004, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (**1990**), (3), 355-62
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



AB Pyridinium dichloromethylides reacted with di-Me maleate to give tetrahydroindolizinedicarboxylates (I; R, R2 = H, Me, Br; R1 = H, Me, Cl, PhCO), which were easily dehydrochlorinated and dehydrogenated to give indolizinedicarboxylates (II, R3 = CO2Me). 4-Picolinium dichloromethylide reacted with Me 3-phenylpropiolate to give II (R = R2 = H, R1 = Me, R3 = Ph) regioselectively. The exptl. results were compared with HMO predictions.

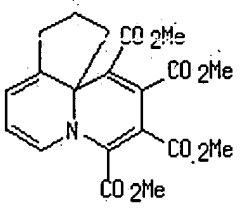
IT **129247-00-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 129247-00-3 HCAPLUS
CN 1H-Benzo[c]quinolizine-3,4-dicarboxylic acid, 10-methyl-1-oxo-, dimethyl ester (9CI) (CA INDEX NAME)



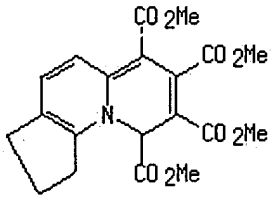
L7 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1985:595974 HCAPLUS
DOCUMENT NUMBER: 103:195974
TITLE: Addition reactions of heterocyclic compounds. Part 81. Products from dimethyl acetylenedicarboxylate with some cycloalkyl[b]pyridines
AUTHOR(S): Abbott, Patrick J.; Acheson, R. Morrin; Choi, Michael C. K.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, OX1 3QU, UK
SOURCE: Journal of Chemical Research, Synopses (**1985**), (6), 169
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:195974
GI



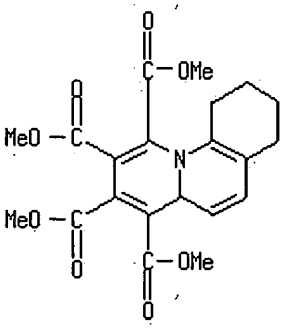
II



III

AB Treatment of cycloalkyl[b]pyridines with MeO2CC≡CCO2Me (I) gave tetra-Me 9aH-quinolizine-1,2,3,4-tetracarboxylates along with other quinolizines and oxoquinolizines. E.g., treatment of 6,7-dihydro-5H-cyclopenta[b]pyridine with I in DMF for 12 days gave tetracarboxylates II and III.

IT **99087-66-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 99087-66-8 HCAPLUS
CN 7H-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a,8,9,10-tetrahydro-, tetramethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1984:610941 HCAPLUS
DOCUMENT NUMBER: 101:210941
TITLE: Addition of trimethylsilyl enol ethers to quinolinium salts: a facile synthesis of methyl

2-(2-oxoalkyl)-1,2-dihydroquinoline-1-carboxylates and their cyclization

AUTHOR(S): Akiba, Kinya; Kobayashi, Toshifumi; Yamamoto, Yohsuke

CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, 730, Japan

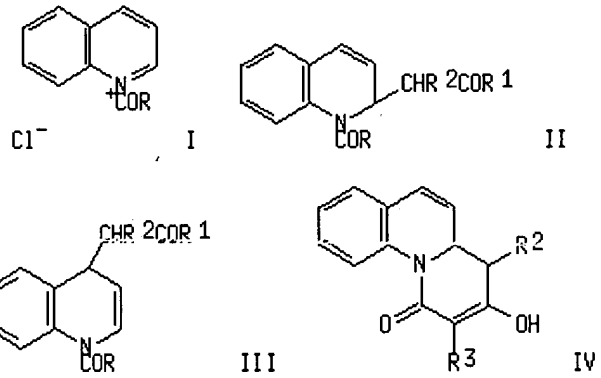
SOURCE: Heterocycles (**1984**), 22(7), 1519-22
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 101:210941

GI

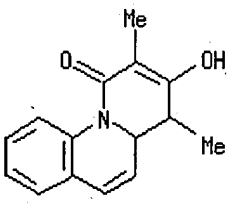


AB Addn. of R2CH:CR1OSiMe3 [R1, R2 = Me, H; Ph, H; Et, Me; OMe, Me; or R1R2 = (CH2)4] to the quinolinium salts I (R = Me, OMe, OEt, OCH2CCl3) gave 85-99% mixts. of quinoline derivs. II and III. II (R - R2 = OMe, Et, Me; OMe, Me, H) were treated with NaH to give the benzoquinolizine derivs. IV (R2 = Me, Me; H, H; resp.).

IT **92637-11-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 92637-11-1 HCAPLUS

CN 1H-Benzo[c]quinolizin-1-one, 4,4a-dihydro-3-hydroxy-2,4-dimethyl- (9CI) (CA INDEX NAME)



L7 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1983:612524 HCAPLUS

DOCUMENT NUMBER: 99:212524

TITLE: 1,2-Polymethyleneketocyanoaza heterocycles

INVENTOR(S): Volovenko, Yu. M.; Babichev, F. S.; Pustovit, Yu. M.

PATENT ASSIGNEE(S): Kiev State University, USSR

SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1983, (25), 88.
CODEN: URXXAF

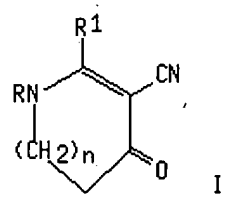
DOCUMENT TYPE: Patent

LANGUAGE: Russian

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

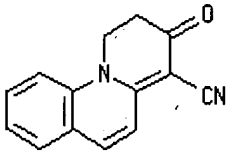
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1027166	A1	19830707	SU 1981-3339358	19810911 <--

PRIORITY APPLN. INFO.: SU 1981-3339358 19810911
OTHER SOURCE(S): CASREACT 99:212524
GI



I

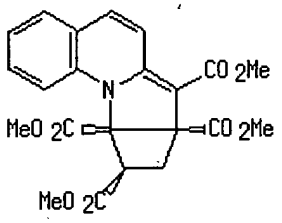
AB Compds. I (RR1 = o-C6H4CH:CH, o-C6H4C6H4-o, o-C6H4NMe; n = 1, 2) are prepd. by treating RN:CR1CH(CN)CO(CH2)nCH2R2 (R2 = Cl, Br) with org. bases under reflux.
IT **87905-54-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 87905-54-2 HCAPLUS
CN 1H-Benzo[c]quinolizine-4-carbonitrile, 2,3-dihydro-3-oxo- (9CI) (CA INDEX NAME)



L7 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1980:110806 HCAPLUS
DOCUMENT NUMBER: 92:110806
TITLE: Addition reactions of heterocyclic compounds. Part 69. Further studies of reactions between 2-alkylquinolines and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. Morrin; Procter, Garry
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, OX1 3QU, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1979**), (9), 2171-9
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



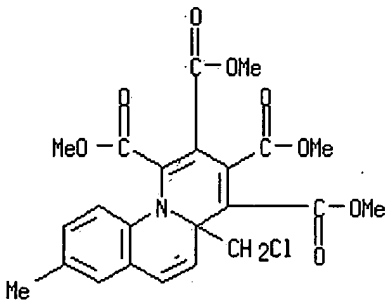
II

AB The reactions of MeO2CC≡CCO2Me (I) with Et quinoline-2-acetate, other quinolines with activated 2-Me groups, and 2-acetoxyquinoline were studied spectroscopically. Mechanistic schemes are proposed for the formation of cyclobutapyrroloquinoline II by the cycloaddn. reaction of 2-methylquinoline with I. Reactions of II, based on its previously reported azepine structure (A. et al., 1968), are reinterpreted using 13C NMR data.

IT **72813-97-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 72813-97-9 HCAPLUS

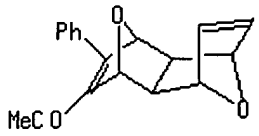
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-(chloromethyl)-8-methyl-, tetramethyl ester (9CI) (CA INDEX NAME)



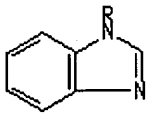
L7 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

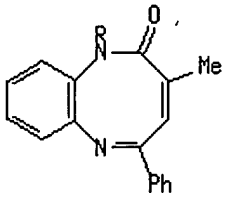
ACCESSION NUMBER: 1979:491477 HCAPLUS
DOCUMENT NUMBER: 91:91477
TITLE: Addition reactions of heterocyclic compounds. Part 67. Products from 1-phenylbut-1-yn-3-one with various heterocycles, and from dimethyl acetylenedicarboxylate with some 2-substituted pyridines
AUTHOR(S): Acheson, R. Morrin; Wallis, John D.; Woollard, John
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1979**), (3), 584-90
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



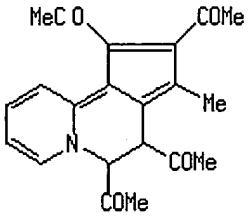
II



III



IV



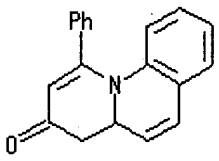
V

AB Treating PhC≡CCOMe (I) with 1-alkylpyrroles effected dimerization, whereas with furan, the adduct II was formed. With 3-methylpyridine and quinoline, I gave dihydroquinolizinones. Treating I with benzimidazole (III; R = H) gave mainly Z-III (R = CPh:CHCOMe) with some of the corresponding E-isomer whereas with III (R = Me, Et, CH2Ph), ring expansion to benzodiazocinones IV took place. Treating 1-(2-pyridyl)butan-2-one with MeO2CC≡CCO2Me gave quinolizine V, whereas other pyridines gave quinolizines, azepines, and indolizines.

IT **71127-12-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 71127-12-3 HCAPLUS

CN 3H-Benzo[c]quinolizin-3-one, 4,4a-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



L7 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

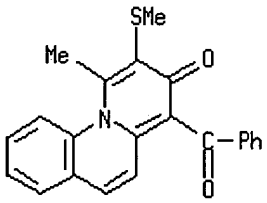
ACCESSION NUMBER: 1976:59142 HCAPLUS
DOCUMENT NUMBER: 84:59142
TITLE: Stable sulfur ylides. IV. Reaction of dimethylsulfonium acetylmethoxycarbonylmethylide and dimethylsulfonium diacetylmethylide with quinoline 1-oxide
AUTHOR(S): Watanabe, Mitsuaki; Kodera, Makoto; Kinoshita, Toshio; Furukawa, Sunao
CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (**1975**), 23(11), 2598-604
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Me2S+C-(COMe)CO2Me reacted with quinoline 1-oxide (I) in the presence of BzCl to give pyrrolo[1,2-a]quinolines II(R = H, 2-quinolyl)and III. Similarly, Me2S+C-(COMe)2 and 3H-pyrido[1,2-a]quinoline IV.

IT **58346-57-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

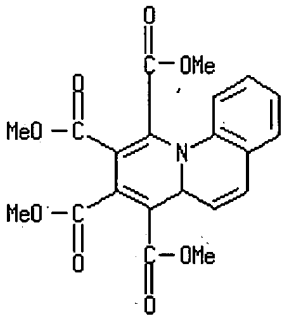
RN 58346-57-9 HCAPLUS
CN 3H-Benzo[c]quinolizin-3-one, 4-benzoyl-1-methyl-2-(methylthio)- (9CI) (CA INDEX NAME)



L7 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1975:111924 HCAPLUS
DOCUMENT NUMBER: 82:111924
TITLE: Photoisomerization of benzo[c]quinolizines. Isolation of the first 2H-quinolizines derivative
AUTHOR(S): Plunkett, A. Owen
CORPORATE SOURCE: Dep. Chem., Portsmouth Polytech., Portsmouth, UK
SOURCE: Tetrahedron Letters (**1974**), (48), 4181-2
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Irradn. of tetra-Me 4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylate (I) in C6H6 gave the 3H-benzo[c]quinolizine II, the 1H tautomer of I, a benzo[c]indolizine, and a red dimer.
IT 26593-23-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(isomerization of, photochem.)
RN 26593-23-7 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

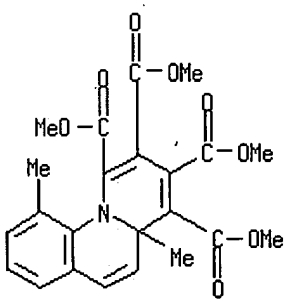


L7 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1973:491951 HCAPLUS
DOCUMENT NUMBER: 79:91951
TITLE: Addition reactions of heterocyclic compounds. LII. Adducts from substituted 2-methylquinolines and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. Morrin; Nisbet, Donald F.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxf., Oxford, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1973**), (13), 1338-46
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Mono-, di-. and trimethylquinolines with MeO2CC≡CCO2Me gave dark red adducts of two types, thought to be geometric isomers. E.g. 2-methylquinoline with MeO2CC≡CCO2Me gave a mixt. contg. hexa-Me 6,7,7a,8-tetrahydrobenzo[f]cyclopenta[a]quinolizine-6,7,7a,8,9,-10-hexacarboxylate (I) and an isomer. Other products from these reactions included benzo[c]quinolizine-, azepino [1,2-a]quinoline-, and 2-propenylquinolinecarboxylates. 2,8-Dimethyl- and 2,4,6,8-tetramethylquinoline also gave 2-[tris(methoxycarbonyl)phenyl]quinolines.
IT **49616-77-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 49616-77-5 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a,10-dimethyl-, tetramethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN
Full Text | Citing References
ACCESSION NUMBER: 1972:114251 HCAPLUS
DOCUMENT NUMBER: 76:114251
TITLE: High-modulus-elasticity polycarbonate compositions
INVENTOR(S): Jackson, Winston J., Jr.; Caldwell, John R.
PATENT ASSIGNEE(S): Eastman Kodak Co.
SOURCE: U.S., 10 pp. Continuation-in-part of U.S. 3,386,935 (CA 69;28318h).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3625877	A	19711207	US 1968-696124	19680108 <--

PRIORITY APPLN. INFO.: US 1968-696124 19680108
AB Addns. of 2-50% stiffening agent, such as polystyrene thioglycol [34568-07-5] with mol. wt. 444-3400, abietyl alc. (I) [666-84-2] hydrogenated I, and mono and diesters obtained from the condensation of unsatd. and hydrogenated I with mono-and dicarboxylic acids contg. .leq.19 C atoms, to bisphenol polycarbonates and polyesters increased the modulus, tensile strength, and hardness of the polymers while decreasing

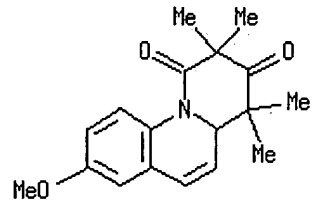
elongation. Thus, a bisphenol A-phosgene copolymer [25971-63-5] was mixed with 20% Me abietate [127-25-3] and the compn. was injection molded into articles with modulus 4.7 .tim. 105 psi, break strength 12,700 psi and elongation at break 4%. Articles molded from a polymer compn. contg. 20% di-Bu phthalate had modulus 3.0 .tim. 105 psi, break strength 7000 psi, and elongation at break 14%.

IT **16977-99-4**

RL: USES (Uses)
(stiffening agents, for polyesters)

RN 16977-99-4 HCAPLUS

CN 1H-Benzo[c]quinolizine-1,3(2H)-dione, 4,4a-dihydro-8-methoxy-2,2,4,4-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:540662 HCAPLUS
DOCUMENT NUMBER: 75:140662
TITLE: Addition reactions of heterocyclic compounds. XLV. New azepines from substituted 2-methylquinolines and dialkyl acetylenedicarboxylates
AUTHOR(S): Acheson, R. M.; Nisbet, D. F.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1971**), (19), 3291-6
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

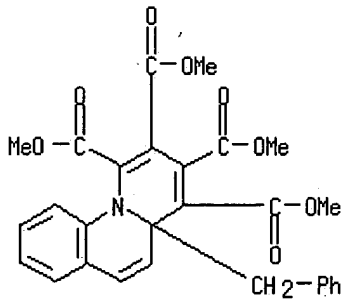
AB 3- and 4-Substituted 2-methylquinolines (e.g. 2,4-dimethylquinoline) reacted with MeO2CC≡CCO2Me to give tetra-Me 10,11-dihydroazepino-[1,2-a]quinoline-7,8,9,10-tetracarboxylates (e.g. I) and tetra-Me 4a-methyl-4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylates (e.g. II). 2-Benzylquinoline reacted similarly, but 2-ethyl-and 2,3-dimethylquinoline gave mixts. of the azepinoquinoline-7,8,9,10- and -7,8,9,11-tetracarboxylates.

IT **33898-14-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 33898-14-5 HCAPLUS

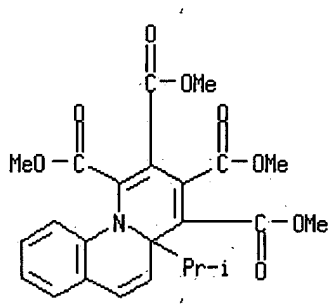
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-benzyl-, tetramethyl ester (8CI) (CA INDEX NAME)



L7 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:540657 HCAPLUS
DOCUMENT NUMBER: 75:140657
TITLE: Addition reactions of heterocyclic compounds. XLIV. Synthesis and photoisomerism of some quinolizine esters
AUTHOR(S): Acheson, R. M.; Stubbs, J. K.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1971**), (19), 3285-91
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB D labeling showed that the thermal rearrangement of tetra-Me 4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylate into the 1H-isomer is an intramol. process whereas the photochem. conversion involves D exchange with MeOH as solvent. MeO2CC≡CCO2Me reacted with 2-isopropyl- and 2-styrylquinoline, 2,3-dihydro-1H-cyclopenta[b]quinoline, and 1,2,3,4-tetrahydroacridine to give tetra-Me 4a-isopropyl- and 4a-styryl-4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylates, tetra-Me 6,7-dihydro-5H-benzo[c]cyclopenta[j]quinolizine-1,2,3,4-tetracarboxylate (I), and tetra-Me 5,6,7,8-tetrahydrodibenzo[cj]quinolizine-1,2,3,4-tetracarboxylate (II), resp. Irradn. of these quinolizines and other quinolizines with bridgehead H atoms or alkyl groups caused migration of the bridgehead group to C-1 in sterically favorable cases, sometimes with the formation of pyrroloazepines.
IT **33922-40-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and photochem. rearrangement of)
RN 33922-40-6 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-isopropyl-, tetramethyl ester (8CI) (CA INDEX NAME)



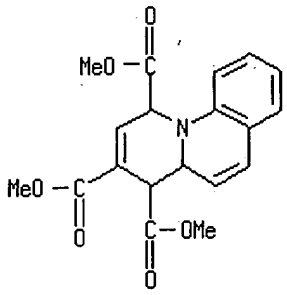
L7 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:529616 HCAPLUS
DOCUMENT NUMBER: 75:129616
TITLE: Addition reactions of heterocyclic compounds. XLVI. Reactions of acetylenic esters with pyridines in the presence of proton donors, and with alkyl 3-(2-pyridyl)-trans-acrylates
AUTHOR(S): Acheson, R. M.; Woollard, J. McK.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1971**), (19), 3296-305
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 3,5-Dimethylpyridine and HC≡CCO2Me gave Me 1,2-dihydro-1-[trans-2-(methoxycarbonyl)vinyl]-3,5-dimethyl-2-pyridinepropiolate. Pyridine and its 3-Me and 3,5-di-Me derivs. reacted with HC≡CCO2Me-MeOH to give Me 1,2-dihydro-2-methoxy-1-pyridineacrylates, and with HC≡CCO2-Me-H2O to give Me 1-pyridineacrylates contg. a (methoxycarbonylvinyloxy)(methoxycarbonyl)vinyl side chain. Reaction of 3,5-dimethylpyridine with HC≡CCO2Me-PhOH gave a 1:19 mixt. of Me cis and trans-phenoxyacrylates. Et 3-(2-pyridyl)-trans-acrylate with acetylenic mono- and diesters gave 4H-quinolizines via a spiro intermediate, with apparent migration of an ester group.

IT **33802-96-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 33802-96-9 HCAPLUS
CN 1H-Benzo[c]quinolizine-1,3,4-tricarboxylic acid, 4,4a-dihydro-, trimethyl ester (8CI) (CA INDEX NAME)



L7 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:498516 HCAPLUS
DOCUMENT NUMBER: 75:98516
TITLE: Ketenes. XIV. Adducts of dimethylketene with C:N compounds
AUTHOR(S): Martin, James Cuthbert; Brannock, Kent C.; Burpitt, Robert D.; Gott, P. Glenn; Hoyle, V. A., Jr.
CORPORATE SOURCE: Tennessee Eastman Co. Div., Eastman Kodak Co., Kingsport, TN, USA
SOURCE: Journal of Organic Chemistry (**1971**), 36(16), 2211-15
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal

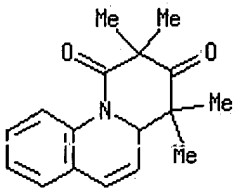
LANGUAGE: English

AB The structures of the 2:1 adducts of dimethylketene with azomethines and N-heterocycles were incorrectly assigned in the early literature. These materials are oxazinone derivs. rather than piperidinediones. For some C.N compds., bulky substituents on the N of the azomethine and use of solvents of low polarity favor β-lactam formation at the expense of oxazinone.

IT **6082-64-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 6082-64-0 HCAPLUS

CN 1H-Benzo[c]quinolizine-1,3(2H)-dione, 4,4a-dihydro-2,2,4,4-tetramethyl- (7CI, 8CI) (CA INDEX NAME)



L7 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1970:3340 HCAPLUS

DOCUMENT NUMBER: 72:3340

TITLE: Addition reactions of heterocyclic compounds. XLI. Photolysis of some quinolizine esters

AUTHOR(S): Acheson, Richard M.; Stubbs, J. K.

CORPORATE SOURCE: Dep. Biochem., Oxford, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (**1969**), (17), 2316-19
CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

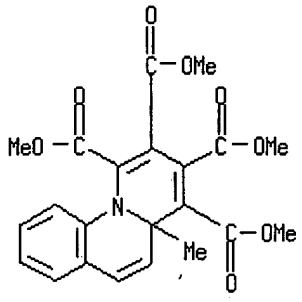
GI For diagram(s), see printed CA Issue.

AB The irradn. of some tetramethyl 9aH-quinolizine-1,2,3,4-tetracarboxylates gave low yields of pyrrolo[1,2-a]azepines (e.g. I); similar 4aH-benzo[c]quinolizines gave corresponding 1H-isomers and other compds. The NMR and mass spectra and mode of formation of the products are discussed.

IT **17260-83-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photolysis of)

RN 17260-83-2 HCAPLUS

CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-methyl-, tetramethyl ester (7CI, 8CI) (CA INDEX NAME)



L7 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1968:428318 HCAPLUS
DOCUMENT NUMBER: 69:28318
TITLE: High modulus polyester and polycarbonate compositions
INVENTOR(S): Jackson, Winston J., Jr.; Caldwell, John R.
PATENT ASSIGNEE(S): Eastman Kodak Co.
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3386935	A	19680604	US 1966-561370	19660629 <--

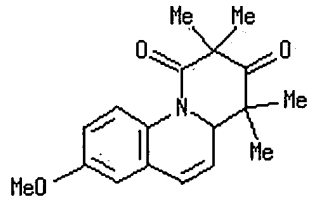
PRIORITY APPLN. INFO.: US 1966-561370 19660629

GI For diagram(s), see printed CA Issue.

AB Antiplasticizers increase the modulus, tensile strength, m.p., heat-distortion temp., and hardness of polycarbonate and polyester compns. making them useful for the prepn. of films, fibers, and shaped articles. Thus, to a polycarbonate with inherent viscosity 1.01 prepd. from bisphenol A and COCl2 was added 20 wt. % polystyrylene glycol (I) (mol. wt. 500). The resulting compn. had modulus 4.6 × 105 psi., break strength 13,500 psi. and 4% elongation at break, compared with the same polycarbonate with no additive or with conventionally used dibutyl phthalate, resp., modulus 3.0-3.3 × 105, 3.0 × 105 psi., break strength 9000-9500, 7000 psi.; and 20-90%, 14% elongation at break. Similar tests were performed on other polycarbonates and additives. Polyesters were also studied.

IT **16977-99-4**
RL: USES (Uses)
(as antiplasticizer, for polyesters)

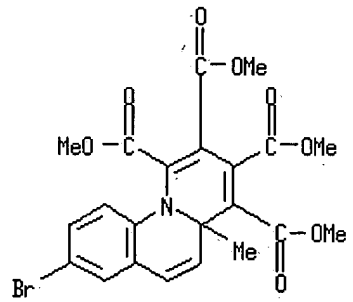
RN 16977-99-4 HCAPLUS
CN 1H-Benzo[c]quinolizine-1,3(2H)-dione, 4,4a-dihydro-8-methoxy-2,2,4,4-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1968:68849 HCAPLUS
DOCUMENT NUMBER: 68:68849
TITLE: Addition reactions of heterocyclic compounds. XXX. Acetylenedicarboxylic esters with benzopyridines possessing activated methyl groups
AUTHOR(S): Acheson, Richard M.; Gagan, J. M. F.; Harrison, Derek R.
CORPORATE SOURCE: Dep. Biochem., Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1968**), (4), 362-78
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Dimethyl and diethyl acetylenedicarboxylate, with 2-methylquinoline and some derivs., 1-methylisoquinoline, and 6-methylphenanthridine, give dihydroazepines with the migration of an ester group; benzoquinolizines, such as I, and other products are also formed. The N.M.R. spectra of the ethoxycarbonyldihydroazepines and some derivs. were fully analyzed. Hydrogenation, protonation, bromination, hydrolysis, and oxidn. of the azepines were investigated, and a scheme for their formation is proposed. The N.M.R. spectra for some benzoquinolizines are tabulated. 36 references.
IT **17247-10-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 17247-10-8 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 8-bromo-4a-methyl-, tetramethyl ester (8CI) (CA INDEX NAME)



L7 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

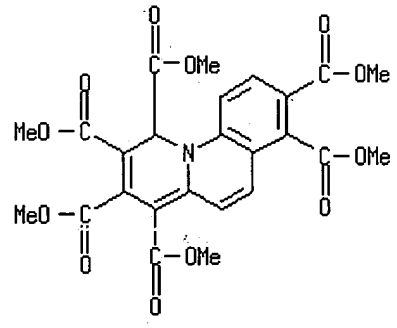
ACCESSION NUMBER: 1968:68845 HCAPLUS
DOCUMENT NUMBER: 68:68845
TITLE: Addition reactions of heterocyclic compounds. XXXIII. New adducts from some pyridines and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, Richard M.; Foxton, Michael W.; Hands, Anthony R.
CORPORATE SOURCE: Dep. Biochem., Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1968**), (4), 387-9
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1,2- and 1,3-Adducts were obtained from both 2-phenyl- and 2-vinylpyridines with dimethyl acetylenedicarboxylate, and their structures deduced largely from N.M.R. spectra. The adducts from 2-phenylpyridine possess one very high-field ester resonance due to shielding by the phenyl ring.

IT **17880-55-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 17880-55-6 HCAPLUS

CN 1H-Benzo[c]quinolizine-1,2,3,4,7,8-hexacarboxylic acid, hexamethyl ester (8CI) (CA INDEX NAME)



L7 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1968:39445 HCAPLUS
DOCUMENT NUMBER: 68:39445
TITLE: Syntheses of heterocycles. XCIX. Quinolizines and indolizines. 4. Synthesis of hydroxybenzoquinolizinones
AUTHOR(S): Kappe, Thomas
CORPORATE SOURCE: Univ. Graz, Graz, Australia
SOURCE: Monatshefte fuer Chemie (**1967**), 98(6), 2148-56
CODEN: MOCHAP
DOCUMENT TYPE: Journal
LANGUAGE: German

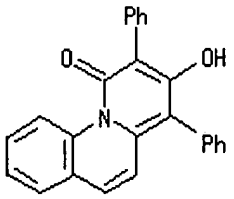
GI For diagram(s), see printed CA Issue.

AB 2-Alkylquinolines (I) react with monosubstituted 2,4,6-trichlorophenyl malonates CHR(CO2C6H2Cl3)2 (II) at 250° to give derivs. of hydroxybenzo[c] quinolizinone. The reaction of quinaldine itself with II leads to pyronoquinolizinones (III). The reaction of II with 1-methylisoquinoline yields 2-hydroxy-4H-benzo[a]quinolizin-4-ones, and with 6-alkylphenanthridines dibenzo[a,c]quinolizinones are obtained. Carbon suboxide (C3O2) is added readily to ethyl 2-quinolylacetate yielding 4-ethoxycarbonyl-3-hydroxy-1H-benzo[c]quinolizin-1-one.

IT **16956-10-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 16956-10-8 HCAPLUS

CN 1H-Benzo[c]quinolizin-1-one, 3-hydroxy-2,4-diphenyl- (8CI) (CA INDEX NAME)



L7 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

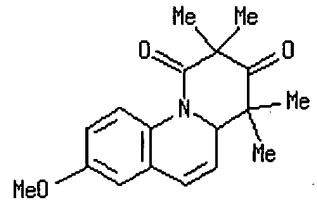
Full Text | Citing References

ACCESSION NUMBER: 1967:464959 HCAPLUS
DOCUMENT NUMBER: 67:64959
TITLE: Antiplasticization. II. Characteristics of antiplasticizers
AUTHOR(S): Jackson, Winston Jerome, Jr.; Caldwell, John R.
CORPORATE SOURCE: Tennessee Eastman Co., Kingsport, TN, USA
SOURCE: Journal of Applied Polymer Science (**1967**), 11(2), 211-26
CODEN: JAPNAB; ISSN: 0021-8995
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The characteristics of materials which act as antiplasticizers for bisphenol polycarbonates are discussed. Antiplasticizers increase the modulus and tensile strength of polycarbonate films and lower the elongation, while plasticizers decrease the modulus and tensile strength, and, in sufficient quantities, increase the elongation. Films of polycarbonates contg. additives were cast from CH_2Cl_2 onto glass plates [antiplasticizer, modulus ×10-5 (psi.), yield strength (psi.), break strength (psi.), elongation at break (%), Elmendorf trear strength (g./mil) given]: none, 3.0-3.3, 8500-9000, 9000-9500, 20-90, 15; Aroclor 1242 (chlorinated biphenyl), 3.9, -, 9000, 9, -; Aroclor 1254, 4.5, -, 14,200, 4, 24; HO(CHPhCH2O)nH (mol. wt. 500), 4.6, -, 13,500, 4, 22; 1-(2,4-dinitrophenyl)-2-phenylethene, 3.7, -, 9800, 4, 20; 2,2'-dinitrobiphenyl, 4.4, -, 12,000, 4, 22; 3,4-dichlorophenyl benzenesulfonate, 3.8, 10,000, 9300, 11, 21; 2,5-dimethyldiphenyl sulfone, 4.2, 9500, 9700, 15, 21; 2,4-dimethoxydiphenyl sulfone, 4.6, 12,000, 10,200, 12, 19; N,N'-diphenyl-N,N'-ditosylethylenediamine, 4.4, -, 12,300, 5, 19; bis[2,2-dimethyl-3-(m-tolyloxy)propyl] carbonate, 4.3, -, 10,100, 3, -; bis(2,4,6-tribromophenoxyethyl) isophthalate, 4.3, -, 12,700, 5, 24; pentaerythritol tetrakis[α-(3-hydroxy-4-benzoylphenoxy)acetate], 4.3, -, 13,500, 4, 23; Abalyn (Me abietate), 4.7, -, 12,700, 4, 23; 1-isopropylidene-4,4-dimethyl-4,4a-dihydro-1H, 3H,[1,3]oxazino[3,4-a]quinolin-3-one, 4.3, -, 12,700, 5,27; 2,2,4,4-tetramethyl-8-methoxy-4aH-benzo[c]quinolizine-1,3(2H,4H)-dione, 4.3, -, 13,200, 5, 23. Results are also given for di-Me phthalate, di-Bu phthalate, dicyclohexyl phthalate, bis[p-(1,1,3,3-tetramethylbutyl)phenyl]phthalate, and di-Ph phthalate. Cf. CA 63: 11791g.

IT **16977-99-4**
RL: USES (Uses)
(as antiplasticizer for polycarbonates)

RN 16977-99-4 HCAPLUS
CN 1H-Benzo[c]quinolizine-1,3(2H)-dione, 4,4a-dihydro-8-methoxy-2,2,4,4-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

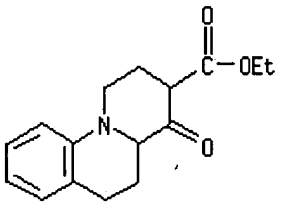
ACCESSION NUMBER: 1966:84768 HCAPLUS
DOCUMENT NUMBER: 64:84768
ORIGINAL REFERENCE NO.: 64:15941e-h,15942c
TITLE: Preparation and chemistry of 10α-estra-4-en-3-ones
AUTHOR(S): Farkas, Eugene; Owen, John M.; Debono, M.; Molloy, R. M.; Marsh, Max M.
CORPORATE SOURCE: Eli Lilly & Co., Indianapolis, IN
SOURCE: Tetrahedron Letters (**1966**), (10), 1023-7
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 54, 21197b. The substituted estra-4,8(10)-dien-3-ones (I, R = H, Me) in alc. hydrogenated with one equiv. H on Pd-BaSO4 or Pd-Al2O3 gave small amts. of the appropriately substituted 5α,10α-estrane (II, R = H, Me) (III, IV) and 20-30% yield of the corresponding 4-en-3-ones (V, R = H, Me) (VI, VII). In general, higher yields (60-80%) of V were obtained by use of 2% Pd-SrCO3 in C6H6 though these alternative conditions were not applicable in some redns. owing to soly. differences. VI, m. 172-3°, λ 245 μ (ε 15,800), showed an optical rotatory dispersion (O.R.D.) curve almost identical with that of the corrected curve for 10α-testosterone. The π-π* portion of the curve indicating the chirality of the chromophore showed a neg. Cotton effect, best accommodated by assumption of half-chair and boat formations for the A and B rings and with cis diaxial 2α,10α protons. The upfield shift of the 18-Me protons at 42 cycles/sec. (cps.) as compared to 50 cps. in the N.M.R. spectrum of 19-nortestosterone (VIII) confirmed the boat conformation of the B ring. VI was readily isomerized to VIII by HCl in CHCl3 or with aq. KOBu. Further confirmation of the structure of VI was obtained by the catalytic hydrogenation of the remaining double bond to give the known III. VI was acetylated in Ac2O-C5H5N to the acetate, m. 143-4°, and oxidn. of VI in C5H5N gave high yields of 10α-estra-4-ene-3,17-dione, m. 162-4°. Metal-ammonia redn. of VI yielded 20% 5α,10α-estran-3-on-17β-ol, together with a 60% yield of the 5β,9α,10α-estrane (IX), m. 121-2°. IX exhibited on O.R.D. curve with neg. Cotton effect [φ] - 1022° (λ 314 mμ, in agreement with octant rule predictions. Hydrogenation of I (R = Me) gave VII, m. 193-5°, λ 243 μ (ε 16,400) together with IV as a by-product. The O.R.D. and N.M.R. spectra of VII showed the salient features of I (R = H). VI showed no androgenic activity but maintained a high pituitary agonadotrophin inhibitory activity. A weak uterotrophic response was also noted.

IT **4527-67-7**, 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-oxo-, ethyl ester, hydrochloride
(prepn. of)

RN 4527-67-7 HCAPLUS

CN 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-oxo-, ethyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)



HCl

L7 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

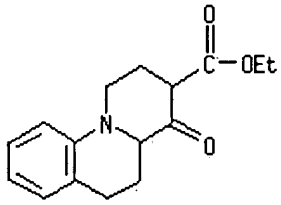
Full Text | Citing References

ACCESSION NUMBER: 1966:84767 HCAPLUS
DOCUMENT NUMBER: 64:84767
ORIGINAL REFERENCE NO.: 64:15941e
TITLE: Azasteroids. III. Approaches to 9-azasteroids
AUTHOR(S): Schleigh, W. R.; Popp, F. D.
CORPORATE SOURCE: Clarkson Coll. of Technol., Potsdam, NY
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1966**), (8), 760-2
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 64, 5161d. Some unsuccessful approaches to 9-azasteroids are described. 3-Deoxy-18-nor-9,15,16-triaza-δ14(15))-estrone has been prepd.

IT **4527-67-7**, 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-oxo-, ethyl ester, hydrochloride
(prepn. of)

RN 4527-67-7 HCAPLUS
CN 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-oxo-, ethyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)



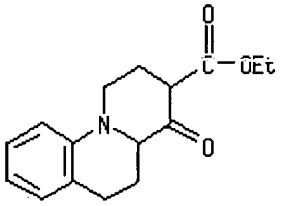
HCl

L7 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1966:84766 HCAPLUS
DOCUMENT NUMBER: 64:84766
ORIGINAL REFERENCE NO.: 64:15941d-e
TITLE: Viridin. V. Structure

AUTHOR(S): Grove, J. F.; McCloskey, P.; Moffatt, J. S.
CORPORATE SOURCE: Imp. Chem. Ind. Ltd., Welwyn, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1966**), (8), 743-7
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. preceding abstr. The structure of viridin (I), C20H16O6, an antifungal metabolic product of Gliocladium virens, is elucidated.
IT **4527-67-7**, 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-oxo-, ethyl ester, hydrochloride (prepn. of)
RN 4527-67-7 HCAPLUS
CN 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-oxo-, ethyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)



HCl

L7 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN
Full Text | Citing References
ACCESSION NUMBER: 1966:35773 HCAPLUS
DOCUMENT NUMBER: 64:35773
ORIGINAL REFERENCE NO.: 64:6613b-h,6614a-h,6615a-h,6616a-b
TITLE: Synthesis of 9-azasteroids. II. Synthesis of β-cyano- and β-carbethoxy-3-and 4-oxo-1,2,3,4,5,6-hexahydrobanzo[c]quinolizines
AUTHOR(S): Jones, G.; Wood, J.
CORPORATE SOURCE: Univ. Keele, UK
SOURCE: Tetrahedron (**1965**), 21(10), 2961-71
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 64, 2048c. The synthesis of 3- and 4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizines with reactive ester or nitrile groups situated so as to allow addn. of a 4th ring (ring D of the final 9-azasteroid) was reported. The previously prepd. oxo ester (I, 12.4 g.) in 100 ml. dry PhMe treated portionwise with 1.3 g. NaH (50% paraffin mull) and the mixt. refluxed 1 hr. with stirring, the cooled soln. treated with 9.63 g. MeI in 25 ml. PhMe and the stirred soln. slowly heated in 1 hr. to boiling, refluxed 2 hrs. and the cooled mixt. dild. with 100 ml. dry Et2O, the filtered soln. evapd. and the brown oil (5.5 g.) sepd. on Al2O3 gave the alkylation product (II), b0.0002 125-30°, and its stereoisomer, b0.0002 140-5°. Alternative routes to the non-enolizable oxo ester (III) were investigated. EtOCH2CH2OH (300 g.) and 350 g. PBr3 mixed slowly below 80° and stirred 1 hr. poured into 500 ml. ice-H2O and the washed and dried bromide distd. at 50 mm.

gave 285 g. EtOCH2CH2Br. K (40.4 g.) in 800 ml. dry Me3COH stirred 30 min. at 50° with 150 g. MeCH(CO2Et)2 and the mixt. refluxed 2 hrs. with stirring with 178 g. EtOCH2CH2Br, the solvent evapd. and the residue treated at 0° with 400 ml. ice-H2O and Et2O yielded 161 g. EtOCH2CH2CMe(CO2Et)2 (IV), b10 130-2°. The ester (26 g.) in 200 ml. abs. alc. satd. with HBr and kept 16 hrs., refluxed 2 hrs. and evapd. in vacuo, the residual mixt. poured into 50 ml. ice-H2O and the aq. layer basified with NaHCO3, extd. with Et2O and the dried ext. distd. yielded 74% substantially pure BrCH2CH2CMe(CO2Et)2 (V), b11 138-40°. IV (102 g.) in 600 ml. 33% HBr boiled 6 hrs. with periodic distn. of EtBr, and removal of HBr in vacuo, HBr distd. in vacuo and the distillate neutralized, satd. with NaCl and extd. with Et2O, the extd. lactone and the carboxylactone distn. residue combined, heated 1 hr. at 200° and distd. yielded 73% 2-methyl-4-butyrolactone (VI),b11 81°. VI (32 g.) in 80 ml. abs. alc. satd. with HBr at 0° and the mixt. kept 24 hrs. at 20°, resatd. with HBr and kept 12 hrs. before pouring onto 120 g. ice, the ester layer and Et2O washings of the aq. layer combined and the washed and dried soln. distd. gave material, b1.0 45-50°, contaminated with 10% VI. Further washing with H2O and distn. gave pure BrCH2CH2CHMeCO2Et (VII), b1.0 47°. VII (49 g.), 24 g. Et 1,2,3,4-tetrahydroquinaldinate, 32.3 g. anhyd. K2CO3, and 1 g. KI heated 6 hrs. at 160-70° with vigorous stirring and the cooled mixt. treated with cold H2O and CHCl3, the CHCl3 layer dried and distd. at 10 mm. to give 12.1 g. VI and the pressure reduced gave 8.9 g. fraction, b0.18 104-40°. Further distn. at 0.0006 mm. yielded 61% material, b0.0006 140-60°, redistd. to give pure Et N-(3-ethoxycarbonylbutyl)-1,2,3,4-tetrahydroquinaldinate (VIII), b0.0006 154-6°. VIII (11.5 g.), 21.5 g. V, and 10.6 g. anhyd. K2CO3 heated 7 hrs. at 160° with stirring and the product fractionally distd. gave mainly VIII, 2-ethoxycarbonyl-2-methyl-4-butyrolactone, and 8% required Et N-[3,3-bis(ethoxycarbonyl)butyl]-1,2,3,4-tetrahydroquinaldinate, b0.0006 150°. VIII (8.65 g.) in 60 ml. dry xylene added in 30 min. to KOBu-tert (from 1.09 g. K) in 50 ml. refluxing xylene with distn. of evolved BuOH, the cooled mixt. dild. with 300 ml. dry Et2O and the hygroscopic K salt (6.0 g.) converted to the unstable base gave the acyloin (IX), HCl salt, m. 96-7°. Since the major difficulty in alkylating the cyclic ester I appeared to be competitive N-alkylation the basicity of the N was deactivated by nitration in the para-position using N2O4 in CCl4 according to Schaarschmidt et al. (CA 19, 2036). Et N-(3-ethoxycarbonylpropyl)-1,2,3,4-tetrahydroquinaldinate (X, R = H, 5.0 g.) in 50 ml. dry CCl4 at -5° stirred vigorously with 1.6 g. powd. CaCO3 with addn. of 1.45 g. N2O4 in 20 ml. CCl4 and the mixt. stirred 3 hrs. at -5°, warmed slowly and filtered at 20°, washed with 100 ml. cold 3N HCl, satd. aq. NaHCO3, and H2O and the dried soln. evapd. yielded 83% brown oil. A sample distd. in a bulb tube gave X (R = NO2) (XI), b0.001 200-10°. I (4.77 g.) in 100 ml. CCl4 at -5° stirred 30 min. with addn. of 1.69 g. N2O4 in 40 ml. ice-cold CCl4 and the mixt. stirred 3 hrs., the soln. decanted at 20° and the decantation and CCl4 washings evapd. yielded 24% solid. Recrystn. of a sample gave the nitro oxoester (XII, R = H) (XIII), m. 126-9°. XIII (1.35 g.) in 30 ml. PhMe added slowly to 50 ml. refluxing PhMe contg. of KOBu-tert (from 0.18 K) and the mixt. refluxed 30 min., the cooled mixt. treated with 1.2 g. MeI in 20 ml. PhMe and the mixt. slowly heated and refluxed 3 hrs., cooled and the filtered soln. evapd. gave an unstable gum, corresponding to the expected methylated compd. XII (R = Me). XI (0.66 g.) in 100 ml. alc. hydrogenated over 0.1 g. prereduced PtO2 with adsorption of 3 molar equivs. H gave 0.61 g. brown oil, distd. to give the amino diester X (R = NH2), b0.0003 185-95°. The previously synthesized cyano ester (XIV, 8.16 g.) in 75 ml. xylene added in 1 hr. with stirring to 2.25 g. NaOEt in 75 ml. boiling xylene with slow distn.,

the stirred mixt. refluxed 1 hr. and distd. to vapor temp. 138°, the ice-cold suspension dild. with 100 ml. each of Et2O and H2O and the org. layer extd. with 100 ml. N aq. NaOH, the combined aq. layers adjusted with 5N HCl at 0° to pH 6 and extd. with CHCl3, the residue on evapn. (6.41 g. brown gum) purified by regeneration from the HCl salt and a sample distd. gave 3-cyano-4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine, b0.003 180°; HCl salt, m. 163° (decompn.). Nitration of the cyano ketone gave an extremely insol. brown solid which has not been characterized. The major difficulty in synthesis of 4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine derivs. appeared to be inherent instability of systems which are formally analogous to 3-oxo-N-phenylpiperidine and synthesis of the probably more stable 3-oxo derivs. was undertaken. Attempts to synthesize the potentially useful intermediate tricyclic oxo ester (XV, R = H) (XVI) were undertaken. The initial approach was that of cyclization of the diester, Et 1-(2-ethoxycarbonylethyl)-1,2,3,4-tetrahydro-2-quinolyl acetate (XVII). Abs. alc. (300 ml.) and 4 ml. H2O contg. 29.4 g. 2-quinolylacetonitrile (from 2-chloromethylquinoline HCl salt) satd. with HCl at 60° and boiled 3 hrs., the chilled mixt. filtered and the residue on evapn. in vacuo treated with ice-cold satd. aq. NaHCO3, extd. with Et2O and the product distd. yielded 76% Et 2-quinolylacetate, b0.5 136-7°. The acetate (36.65 g.) in 250 ml. AcOH hydrogenated over prereduced PtO2 with 2 moles H and the residue on evapn. treated with aq. NaHCO3 and Et2O, the Et2O layer dried and distd. yielded 92% Et 1,2,3,4-tetrahydro-2-quinolylacetate (XVIII), b0.6 130-8°; 1-benzoyl deriv., m. 96.5-7.0° (ligroine). XVIII (10 g.), 16.42 g. BrCH2CH2CO2Et (b2.5 44°), 9.5 g. finely ground K2CO3, and 0.38 g. KI heated 4 hrs. at 140° under a short air condenser and the cooled mixt. treated with H2O and Et2O, the Et2O layer and washings dried and evapd., the residual oil distd. at 12 mm. to give 4 g. BrCH2-CH2CO2Et and at 0.003 mm. gave 1.7 g. XVIII and 63% yield of XVII, b0.003 145-60°, redistd. to give a sample, b0.003 161°. XVII (12.0 g.) cyclized with EtONa (from 0.95 g. Na in 200 ml. xylene) and the chilled (0°) mixt. treated with 100 ml. H2O, the aq. layer adjusted to pH 6.5 and dild. with Et2O, the org. layer and subsequent Et2O exts. combined and evapd. gave 93% viscous orange oil, purified by regeneration from the HCl salt to give the alternative quinazoline (XIX, R = H) (XX); HCl salt, m. 130° (Me2CO-Et2O-HCl). The cyclized Na salt suspension from 6.0 g. XVII treated at 0° with 3.06 g. MeI in 25 ml. xylene, stirred 1 hr. at 20 and 8 hrs. at 60°, the cooled mixt. filtered and the filtrate and Et2O washings evapd., the light-brown oily mixt. (3.86 g.) chromatographed on neutral Al2O3 from ligroine-C6H6 gave XV (R = Me) (XXI), b0.0004 130-4°, and the major isomer (XIX, R = Me) (XXII), b4 150-5°. The light brown oil (2 g., prepd. as above) boiled 6 hrs. in 5N HCl and evapd., the residue treated with aq. NaHCO3 and the free base extd. with Et2O yielded 73% 2-methyl-3-oxo-1,2,3,4,-5,6-hexahydrobenzo[c]quinolizine (XXIII), b0.003 130-40°. After equilibration with alc. EtONa the redistd. XXIII showed only the doublet at 0.99 ppm. Further confirmation that XXIII was a mixt. of epimers and not of structural isomers was obtained by hydrolyzing and decarboxylating 0.223 g. of the pure major isomer XXII to give 88% XXIII, practically identical with that obtained from the mixt. of oxo esters XXII. The equilibrated ketone XXIII heated 15 min. at 100° with a molar equiv. of 2,4-(O2N)2C6H3NHNH2 in abs. alc./HBr and the cooled mixt. filtered, the salt taken up in CHCl3 and shaken vigorously with aq. Na2CO3 and H2O, dried and evapd. gave XXIII dinitrophenylhydrazone, m. 195-8°. To identify the ketone and hence to deduce the direction of the Dieckmann cyclization in the di-ester XVII, attempts were made to synthesize XXIII or its isomer 4-methyl-3-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine (XXIV), but attempts to alkylate XVIII with

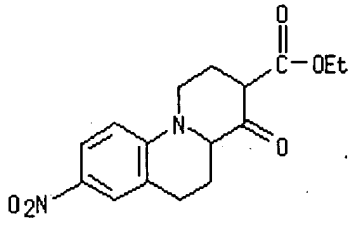
Me2CBrCO2Et were unsuccessful in the production of XXIII. Quinaldyllithium (from 252 g. quinaldine) in Et2O added to 268 g. MeI under gentle reflux and the mixt. refluxed 1 hr., kept 16 hrs. at 20° and treated with 1300 ml. 5N HCl, the acid layer sepd. and the Et2O layer extd. with acid, the combined acid layers basified with NH4OH (d. 0.880) and the bases extd. with Et2O gave 47 g. quinaldine and 57% yield of 2-ethylquinoline, b14 134-5°. A filtered soln. of PhLi (from 90 g. PhBr) added slowly with stirring to 75 g. 2-ethylquinoline in 100 ml. Et2O and the mixt. refluxed 1 hr., the filtered 2-ethylquinolyllithium added in 1 hr. with stirring to 34 g. Et2CO3 in 100 ml. Et2O and the mixt. boiled 3 hrs., the cooled soln. treated with 500 ml. ice-cold 5N HCl, the acid layer and acid exts. neutralized with NH4OH and extd. with Et2O, evapd. and the residue distd. gave 29 g. 2-ethylquinoline b0.05 60-85°, and 15% yield of Et 2-(2-quinolyl)propionate (XXV), b0.05 116°; picrate, m. 137-40° (alc.). XXV (15.8 g.) in 150 ml. AcOH hydrogenated over 0.3 g. prereduced PtO2 with 2 moles H, the filtered soln. evapd. and the residue shaken with aq. NaHCO3 and Et2O, the Et2O ext. dried and distd. gave 85% tetrahydro ester (XXVI) (R = H, R' = CHMeCO2Et) (XXVII), b0.7 134-8°. XXVII (13.9 g.), 21.5 g. BrCH2CH2CO2Et, 12.4 g. K2CO3, and 0.5 g. KI vigorously stirred 6 hrs. at 150° and the cooled product worked up as for XVII gave mainly 8.18 g. XXVII, b0.002 90-120°, and a 73% yield of the diester XXVI (R = CH2CH2CO2Et, R' = CHMeCO2Et) (XXVIII), b0.002 148-54°. XXVIII (6.48 g.) in 50 ml. xylene added slowly to KOCMe3 (from 0.836 g. K) in 75 ml. boiling xylene with slow distn. continued 1 hr., the cooled mixt. treated with 100 ml. ice-H2O and acidified to pH 6, extd. with Et2O and the residue on evapn. gave 2-ethoxycarbonyl-4-methyl-3-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine (XXIX); HCl salt, melting to a thick glass at 50-5°, mobile at 85-90°. XXIX (2.5 g.) boiled 5 hrs. in 50 ml. 5N HCl and the residue on evapn. at 14 mm. treated with satd. aq. NaHCO3 and Et2O, the Et2O ext. dried and distd. gave a ketone, recrystn. from ligroine gave colorless rods, m. 96-7°; 2,4-dinitrophenylhydrazone, m. 153-5°. XXIII and XXIV differed markedly in ir absorption between 1450 and 700 cm.-1 and had retention times of 16.0 and 14.8 min. at 150°. Accordingly the C-methylation decarboxylation product was XXIII, the methylated keto ester XXII and the Dieckmann cyclization of XVII gave the oxo ester XX, unsuitable for further use in a 9-azasteroid synthesis. In view of the high yield obtained in cyclization of the cyano ester XIV it was decided finally to prep. and cyclize the isomeric cyano ester XXVI (R = CH2CH2CO2Et, R' = CH2CN) (XXX). XVIII (18 g.) in 500 ml. dry MeOH satd. with NH3 at 0° and autoclaved 40 hrs. at 100°, the soln. evapd. and the gum triturated with ligroine yielded 85% XXVI (R = H R' = CH2CONH2) (XXXI), m. 98-103°, recrystd. from C5H6 to give a sample m. 103-4°; N-Bz deriv., m. 198-201° (alc.). XXXI (12.5 g.) and 5.93 g. NaCl in 60 ml. ClCH2CH2Cl stirred 15 min. with addn. of 8.93 g. POCl3 in 10 ml. ClCH2CH2Cl, the mixt. warmed and boiled with stirring 12 hrs., the cooled mixt. treated with 8.0 g. NaOH in MeOH and shaken out twice with cold brine, the org. layer dried and distd. yielded 72% XXVI (R = H, R' = CH2CN) (XXXII), b0.06 124-7°; N-Bz deriv., m. 130° (alc.). XXXII (5.0 g.), 10.47 g. BrCH2CH2CO2Et, 6.02 g. K2CO3, and 0.24 g. KI heated 6 hrs. at 140° with stirring, the crude product isolated as for XVII and heated 8 hrs. at 145° with 10.5 g. BrCH2CH2CO2Et and 6 g. K2CO3, worked up again as for XVII to give 1.6 g. XXXII, b0.0006 110-35° and 80% yield of XXX, b0.0006 156-62°, m. 66° (ligroine). XXX (2.96 g.) in 50 ml. xylene added in 1 hr. with stirring to EtONa (from 0.275 g. Na) in 60 ml. boiling xylene and the boiling mixt. stirred 1 hr., worked up as for the cyano ketone from XIV to give 82% light yellow solid, m. 132-8°, recrystd. from alc. to colorless rhombs of the cyano

ketone (XXXIII), m. 135.0-7.5°; HCl salt, m. 133-41° (Me2CO); phenylhydrazone, m. 166-7° (alc.). Since the yields are good throughout the synthesis the intermediate required for elaboration of ring D is available in quantity.

IT **5100-53-8**, 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-8-nitro-4-oxo-, ethyl ester
(prepn. of)

RN 5100-53-8 HCAPLUS

CN 1H-Benzo[c]quinolizine-3-carboxylic acid, 2,3,4,4a,5,6-hexahydro-8-nitro-4-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



L7 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1966:11483 HCAPLUS
DOCUMENT NUMBER: 64:11483
ORIGINAL REFERENCE NO.: 64:2083h,2084a-c
TITLE: Adducts of dimethylketene with C:N-containing compounds
AUTHOR(S): Martin, James C.; Hoyle, V. A., Jr.; Brannock, Kent C.
CORPORATE SOURCE: Tennessee Eastman, Kingsport
SOURCE: Tetrahedron Letters (**1965**), (40), 3589-94
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

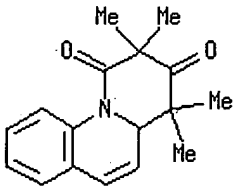
AB Me2C:CO and PhCH:NEt in C6H6 or MeCN gave 95 and 83% yields oxazinone (I), m. 101.5-4.0°, converted by treatment with a catalytic amt. NaOMe to give 92% piperidinedione (II), m. 89.5-91.0°. Treatment of I with excess alc. 1 hr. at 25° gave a quant. conversion to Me2CHCONEtCHPhCMe2CO2Et, b0.4 128-30°, m. 44-5°. On reflux with aq. 10% Na2CO3 30 min., acidification, and recrystn. I yielded 82% Me2CHCONEtCHPhCMe2CO2H, m. 120-1°. II was stable to refluxing alc. and aq. Na2CO3. I treated with NaBH4 in Me3COH gave 22% the isomeric piperidinones (III), m. 188-98°. Redn. of I with LiAlH4 gave 73% the isomeric piperidinols (IV), b0.5 115°, m. 81-6°. These hydride redns. are examples of rearrangement-redns. In each redn. the basicity of the reducing agent brings about the same rearrangement of I as observed with NaOMe. Treatment of III with K2Cr2O7-H2SO4 yielded 95% II. Quinoline and Me2C:CO in MeCN yielded 92% oxazinoquinolinone (V), b0.1 143°, m. 82.0-3.5°. Treatment of V with a catalytic amt. NaOMe brought about rearrangement to give 76% quinolizinedione (VI), m. 84-6°. It would appear that many compds. prepd. by reaction of ketenes with C:N compds. have been assigned piperidinedione structures erroneously.

IT **6082-64-0**, 1H-Benzo[c]quinolizine-1,3(2H)-dione, 4,4a-dihydro-2,2,4,4-tetramethyl-
(prepn. of)

RN 6082-64-0 HCAPLUS

CN 1H-Benzo[c]quinolizine-1,3(2H)-dione, 4,4a-dihydro-2,2,4,4-tetramethyl-

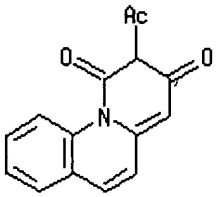
(7CI, 8CI) (CA INDEX NAME)



L7 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

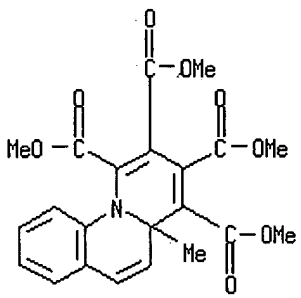
ACCESSION NUMBER: 1963:435553 HCAPLUS
DOCUMENT NUMBER: 59:35553
ORIGINAL REFERENCE NO.: 59:6371e-h
TITLE: Ketene and its derivatives. III. Reaction of diketene with quinoline
AUTHOR(S): Kato, Tetsuzo; Kitagawa, Tsunehiro; Yamamato, Yutaka
CORPORATE SOURCE: Tohoku Univ., Sendai, Japan
SOURCE: Yakugaku Zasshi (**1963**), 83, 267-71
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 59, 2765d. C9H7N(2g.) in 3 ml. C6H6 and 5 ml. diketene (I) refluxed 4 hrs. and the product filtered off gave 2.8 g. C17H13O3N (II), m. 237-8° (decompn.) (MeOH); 0.062 mole C7H7N in 10 ml. C6H6 treated with 0.35 mole ketene, refluxed 3 hrs., kept overnight at 0°, and the product filtered off gave 1.8 g. II, m. 235°(decompn.). II(1.8g.)in 50 ml. BuOH and 0.1 g. 30% Pd-C refluxed 6 hrs., the soln. filtered while hot, and the filtrate concd. to 30 ml. gave 0.75 g. dehydro compd. (III), C17H11O3N, prisms, m. 263-4° (decompn.) (MeOH), the filtrate concd. to 5 ml. and the product filtered off gave 0.36 g. dihydro compd. (IV), C17H15O3N, needles, m. 216-17° (decompn.). III (250 mg.), 30 ml. MeOH, and 10 ml. liquid NH3 in a sealed tube heated 30 hrs. at 50-60° and the product filtered off gave 80 mg. C14H10O3N2 (V), m. 293° (decompn.) (CHCl3), and the mother liquor gave 90 mg. C17H12O2N2.H2O, needles, m. 197-8° (decompn.). III (0.45 g.) in 10 ml. MeOH and 10 ml. 3% NaOH heated 5 min. at 100°, refluxed 30 min., the MeOH removed, the residue neturalized with HCl, and the product extd. with C6H6 gave 100 mg. C17H13O4N (VI), needles, m. 159-60° (Me2CO-H2O). VI (50 mg.) in 3 ml. concd. HCl heated 15 min. at 100°, 10 ml. H2O added, and the product extd. with CHCl3 gave III, m. 264° (decompn.). III (0.37 g.) in 5 ml. MeOH and 15 ml. 3% NaOH refluxed 1 hr. and the product filtered off gave C15H11O3N.0.5H2O, m. 210-11°. Similarly, C5H5N and I or ketene gave C13H11O3N. The above results indicated that the structure of II is VII or VIII.
IT **95516-57-7**, 1H-Benzo[c]quinolizine-1,3(2H)-dione, 2-acetyl- (prepn. of)
RN 95516-57-7 HCAPLUS
CN 1H-Benzo[c]quinolizine-1,3(2H)-dione, 2-acetyl- (7CI) (CA INDEX NAME)



L7 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1963:3230 HCAPLUS
DOCUMENT NUMBER: 58:3230
ORIGINAL REFERENCE NO.: 58:504f
TITLE: The reaction of dimethyl acetylenedicarboxylate with quinaldine
AUTHOR(S): Crabtree, A.; Jackman, L. M.; Johnson, A. W.
CORPORATE SOURCE: Univ. Nottingham, UK
SOURCE: Journal of the Chemical Society, Abstracts (**1962**) 4417-20
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The main product from the reaction of dimethyl acetylenedicarboxylate and quinaldine is formulated as a tricyclic ylide (I) comprising a quinolinium ring with a fused seven-membered cyclic carbanion. The reactions and structure of the tetrabromo addn. product of I are discussed. The other product from the initial quinaldine reaction contains an angular methyl group and is a neutral quinolizine (II) which shows no tendency to rearrange.
IT **17260-83-2**, 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-methyl-, tetramethyl ester
(prepn. of)
RN 17260-83-2 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-methyl-, tetramethyl ester (7CI, 8CI) (CA INDEX NAME)



L7 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1962:403936 HCAPLUS
DOCUMENT NUMBER: 57:3936
ORIGINAL REFERENCE NO.: 57:779a-g
TITLE: Addition reactions of heterocyclic compounds. IX. Benzoquinolizines from isoquinoline and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. M.; Hole, F.

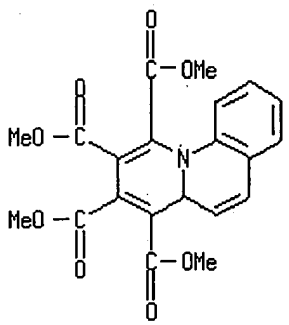
CORPORATE SOURCE: Univ. Oxford, UK
SOURCE: Journal of the Chemical Society, Abstracts (**1962**) 748-52
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 55, 11391g; Diels and Harms, CA 30, 82234. From freshly distd. isoquinoline (I) and MeO2CC:CCO2Me (II) was prepd. as described by D. and H. 77% D. and H's. "1st labile I adduct" (ascribed a different structure by D. and H.), m. 167°; this was now formulated as tetra-Me 11bH-benzo[a] quinolizine1,2,3,4-tetracarboxylate (III). When I was not freshly distd., only about 5% tri-Me benzo[g]indolizine-1,2,3-tricarboxylate (IV) was obtained. I (1 g.) in 5 ml. MeOH mixed with 2 ml. II in 3 ml. MeOH at room temp., kept 2 days, the ppt. collected, and chromatographed on Al2O3 gave IV, m. 154-5° (MeOH). I (8 ml.) in 10 ml. MeOH cooled to -32°, added dropwise to 11 ml. II in 30 ml. MeOH cooled to -32°, the mixt. allowed to rise to 0°, and kept 2 days at 0° gave 2.5 g. IV, identical (m.p., mixed m.p., and infrared absorption spectrum) with IV obtained above. III (1 g.) in 15 ml. AcOH and 5 ml. concd. H2SO4 kept 24 hrs. at 0°, treated with excess solid Na2CO3, and dild. with H2O gave tetra-Me 4H-benzo[a]quinolizine1,2,3,4-tetracarboxylate (V), m. 229-31° (AcOH); this compd. was given a different structure by D. and H. III (0.5 g.) in 5 ml. AcOH contg. 0.5 ml. 60% aq. HClO4 treated with 0.19 g. Br in 1.9 ml. AcOH and kept 16 hrs. gave 1,2,3,4-tetramethoxycarbonylbenzo[a]quinolizium (VI) perchlorate, m. 212° (decompn.) (AcOH). V (0.1 g.) in 5 ml. 1:1 aq.-MeOH treated with 2 g. Br, the mixt. refluxed 5 min., and concd. in vacuo gave VI perbromide, m. 140° (decompn.) (aq. MeOH). III (4 g.) in 30 ml. 1:1 aq.-MeOH treated rapidly with 2 g. Br, refluxed 1 min., and cooled gave 2.2 g. tetra-Me 6,7-dihydro-6-oxo-11bH-benzo[a]quinolizine-1,2,3,4-tetracarboxylate (VII), m. 207° (MeOH). III (4 g.) in 30 ml. 1:1 aq.-MeOH treated with 6 g. Br, refluxed 1 min., and cooled gave 1.7 g. tetra-Me 6 - (o - methoxycarbonylphenyl)pyridine - 2,3,4,5 - tetracarboxylate (VIII), m. 149-50° (MeOH), λ (MeOH) 2800 A. (ε 5800). VII (0.5 g.) in 10 ml. 1:1 aq. MeOH refluxed with 2 g. Br and evapd. in vacuo gave VIII, m.p. and mixed m.p. 149-50° (MeOH). III (1 g.) in 25 ml. MeOH contg. Raney Ni hydrogenated 14 hrs. at 4 atm., filtered, the filtrate concd. in vacuo, the residue shaken with 20 ml. cold MeOH, and the insol. product crystd. from MeOH gave tetra-Me x,x,6,7-tetrahydro-11 bH-benzo[a]quinolizine-1,2,3,4-tetracarboxylate (IX), m. 217°; evapn. of the MeOH ext. gave an isomeric tetrahydro compd., m. 124-6°. V (0.2 g.) in 25 ml. AcOH contg. PtO2 hydrogenated 14 hrs. at 4 atm. gave IX, m. 217°. Tetra-Me 6,7-dihydro11bH-benzo[a]quinolizine-1,2,3,4-tetracarboxylate (X) (0.2 g.) in 20 ml. MeOH contg. Raney Ni hydrogenated 2 hrs. gave IX, m. 217°. III (0.5 g.) in 25 ml. MeOH contg. 5% Pd-C hydrogenated at 4 atm. gave X, m. 179-80° (MeOH). The ultraviolet and infrared absorption spectra data of the adducts, some derivs., and related compds. were tabulated.

IT **26593-23-7**, 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester
(spectrum of)

RN 26593-23-7 HCAPLUS

CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



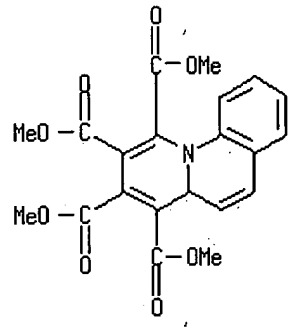
L7 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1961:13423 HCAPLUS
DOCUMENT NUMBER: 55:13423
ORIGINAL REFERENCE NO.: 55:2648g-i,2649a
TITLE: The adducts from quinoline and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. M.; Earl, N. J.; Higham, P.; Richards, R. E.; Taylor, G. A.; Vernon, J. M.
CORPORATE SOURCE: Univ. Oxford, UK
SOURCE: Proc. Chem. Soc. (**1960**) 281-2
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB Quinoline and (MeO2CC≡)2 through a Diels-Alder reaction gave 2 1:2 adducts. The labile adduct (I) isomerized to the stable adduct (II) on heating or treatment with acids. Structures I and II were assigned to these adducts on the basis of similar compds. obtained in the pyridine series (CA 54, 18521a). I was nonbasic in HClO4-HOAc. Its structure was shown by nuclear magnetic resonance (n.m.r.) studies (Van Tamelen, et al., CA 54, 7704b). II did not react with Me2SO4 in MeNO2 at 100° and was monobasic to HClO4 in AcOH. It was a little less basic than tetra-Me 4H-quinolizine-1,2,3,4-tetracarboxylate (the stable pyridine adduct), as approx. 35% HClO4 in MeOH (instead of 8%) was required before the long-wavelength absorption band of the adduct completely disappeared. Diln. with water reversed the change. The hypsochromic shift of the long-wavelength absorption band by approx. 980 A. and other changes in the spectrum observed on acidification were of the magnitude expected for the conversion of the base into the cation.

IT **26593-23-7**, 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester
(prepn. of)
RN 26593-23-7 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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L4           8 S L3
L5         164 S L3 FULL

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L6          42 S L5
L7          33 S L5 AND PD < JANUARY 1998

     FILE 'CAOLD' ENTERED AT 04:46:27 ON 01 OCT 2003

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L8          10 L5
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=> d l8, all, 1-10

L8 ANSWER 1 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA65:7140e CAOLD
TI benzo[c]quinolizinium salts via intramol. cyclization
AU Fozard, Alan; Bradsher, C. K.
IT 2739-76-6 2739-92-6 5330-37-0 5350-12-9 6772-68-5 6772-69-6
6772-70-9 6772-71-0 6772-72-1 6772-73-2 6772-75-4 6772-76-5
6772-79-8 6772-80-1 6772-81-2 6772-82-3 6772-83-4 6772-84-5
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6772-92-5 6772-93-6 6772-94-7 6772-95-8 6772-96-9 6772-97-0
6772-98-1 6773-02-0 6773-05-3 6798-04-5 6798-05-6 6886-46-0
76293-41-9 92102-81-3 92103-32-7 92290-56-7 92290-57-8 93535-01-4
94998-27-3 96279-83-3 **96279-91-3** 96329-85-0 96953-93-4 96984-48-4
96984-49-5 97027-22-0 97437-83-7 97834-69-0 98655-38-0 100299-73-8
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L8 ANSWER 2 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA64:15941e CAOLD
TI azasteroids - (III) 9-azasteroids
AU Schleigh, William R.; Popp, F. D.
TI prepn. and chemistry of 10α-estra-4-en-3-ones
AU Farkas, Eugene; Owen, J. M.; Debono, M.; Molloy, R. M.; Marsh, M. M.
IT 434-22-0 4491-36-5 4527-66-6 **4527-67-7** 4620-34-2 4660-20-2
5233-21-6 5233-22-7 5233-23-8 5233-24-9 5670-42-8 5670-43-9
5670-44-0 5670-45-1 5670-46-2 5670-47-3 5670-51-9 5670-52-0
5670-53-1 5670-54-2 5670-55-3 5670-56-4 5670-57-5 5696-23-1
5696-24-2 6017-86-3

L8 ANSWER 3 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA64:6613c CAOLD
TI synthesis of 9-azasteroids - (II) synthesis of β-cyano- and
β-carbethoxy-3- and 4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizines
AU Jones, Gurnos; Wood, J.
IT 539-74-2 592-55-2 1679-47-6 2213-09-4 5100-50-5 5100-51-6
5100-52-7 **5100-53-8** 5100-54-9 5100-55-0 5100-56-1 5100-57-2
5100-58-3 5100-59-4 5100-61-8 **5100-62-9** **5100-63-0**
5100-64-1 5100-65-2 5100-66-3 5100-67-4 5100-68-5 5100-69-6
5100-70-9 **5100-71-0** 5100-72-1 5100-73-2 5100-74-3 5100-75-4
5100-76-5 **5100-77-6** 5100-78-7 **5161-93-3** 5161-95-5
5161-98-8 5161-99-9 **5569-24-4** 5688-31-3 6166-32-1 14283-09-1

L8 ANSWER 4 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA64:6613b CAOLD
TI synthesis and reactions of 1-carbamoyl- 1 1-oxoindeno[1,2-c]isoquinoline
AU Stowell, James K.
IT 5161-91-1 **5161-92-2** 5580-65-4

L8 ANSWER 5 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA64:2083h CAOLD
TI adducts of dimethylketene with C:N-contg. compds.
AU Martin, James Cuthbert; Hoyle, V. A., Jr.; Brannock, K. C.
IT 598-26-5 4612-76-4 6082-56-0 6082-57-1 6082-58-2 6082-59-3
6082-60-6 6082-61-7 6082-62-8 **6082-64-0**

L8 ANSWER 6 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA64:2048c CAOLD
TI synthesis of 9-azasteroids - (I) attempted synthesis of

4-oxobenzo[c]quinolizidines
AU Jones, Gurnos; Wood, J.
IT 2969-81-5 3153-36-4 4491-26-3 4491-27-4 4491-28-5 4491-29-6
4491-30-9 4491-31-0 4491-32-1 4491-33-2 4491-36-5 4491-38-7
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4627-23-0 4660-20-2 4933-73-7 4933-74-8 96650-09-8

L8 ANSWER 7 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA59:6371e CAOLD
TI heterocyclic quinones from 2,3-dichloro-1,4-naphthoquinone
AU Sartori, Mario F.
TI ketene and its derivs. - (III) reaction of diketene with quinoline
AU Kato, Tetsuzo; Kitagawa, T.; Yamamoto, Y.
IT **95516-57-7** **95771-15-6** **98029-81-3**

L8 ANSWER 8 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA58:504e CAOLD
TI reaction of dimethyl acetylenedicarboxylate with quinaldine
AU Crabtree, A.; Jackman, L. M.; Johnson, A. W.
IT **17260-83-2** 100266-52-2 101358-50-3 107118-15-0

L8 ANSWER 9 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA57:779g CAOLD
TI synthesis of 9, 11, 12, 13, 13a, 14-hexahydro-2,3,6-trimethoxydibenzo[f,h]pyrrolo[1,2-b]isoquinoline
AU Govindachari, Tuticorin R.; Ragade, I. S.; Viswanathan, N.
IT 909-41-1 1971-34-2 4176-23-2 4234-95-1 24892-72-6 **26593-23-7**
30963-47-4 **33922-39-3** 59222-31-0 87101-69-7 93431-38-0 93809-59-7
94005-32-0 94165-06-7 97434-62-3 100088-44-6 100233-74-7 100233-81-6
100266-53-3 101984-30-9 105767-03-1 107160-62-3

L8 ANSWER 10 OF 10 CAOLD COPYRIGHT 2003 ACS on STN
AN CA55:2648g CAOLD
TI adducts from quinoline and dimethyl acetylenedicarboxylate
AU Acheson, Roy M.; Earl, N. J.; Higham, P.; Richards, R. E.; Taylor, G. A.; Vernon, J. M.
IT 762-42-5 **26593-23-7** **33922-39-3** 132753-02-7

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CN 7-Methyl-3-nitrobenzo[c]quinolizinium chloride (7CI) (CA INDEX NAME)
MF C14 H11 N2 O2 . Cl
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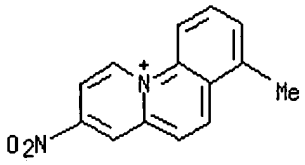

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1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 33922-39-3 REGISTRY
CN 1H-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
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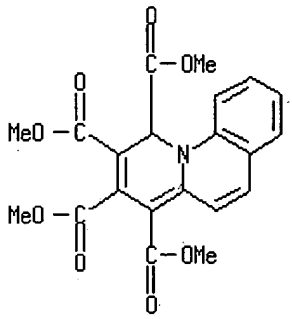

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2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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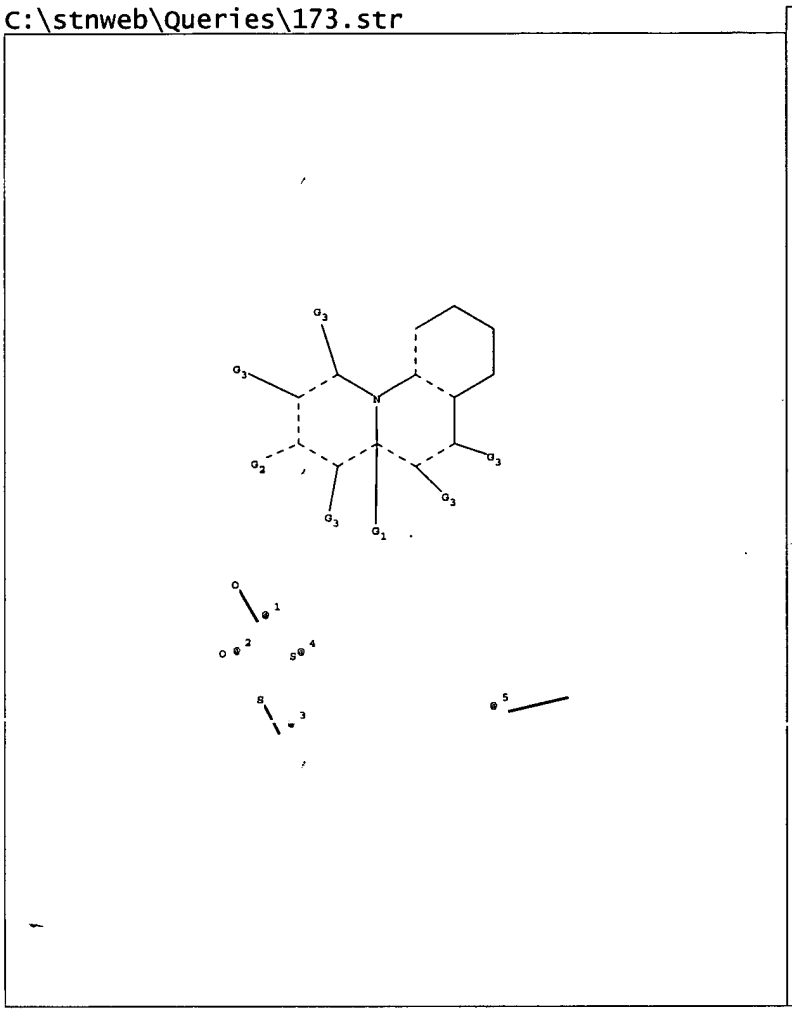

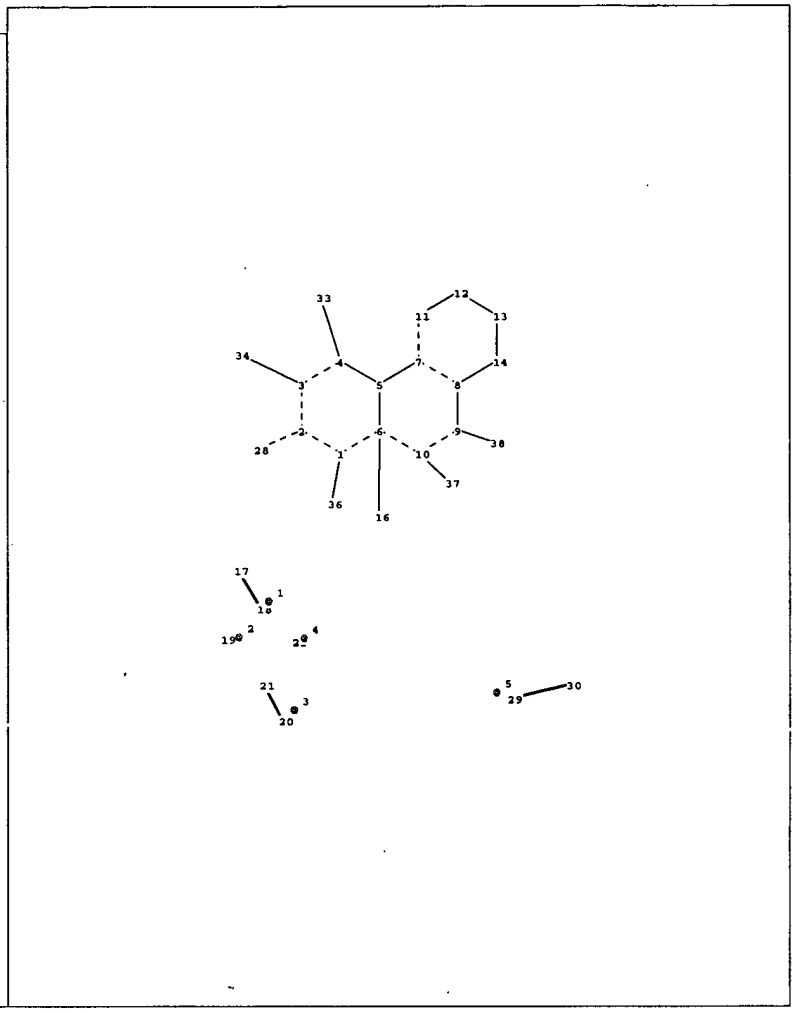

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ring bonds :
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exact bonds :
29-30
isolated ring systems :
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G1:H,Ak

G2:[*1],[*2],[*3],[*4]

G3:H,Ak,Cb,[*5]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS 36:CLASS 37:CLASS 38:CLASS

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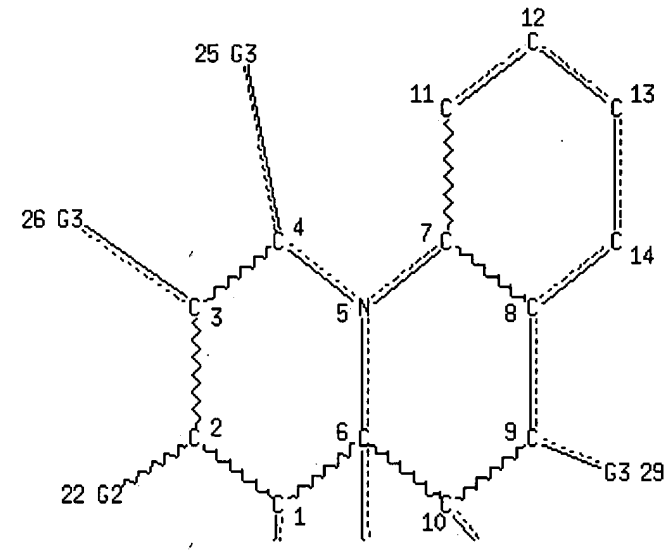

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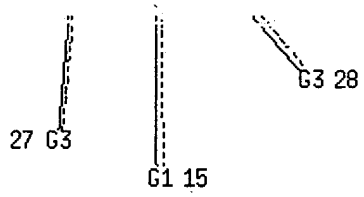

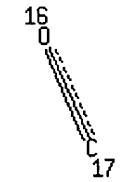

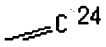

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Page 3-B
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DEFAULT ECLEVEL IS LIMITED

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STEREO ATTRIBUTES: NONE


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SAMPLE SCREEN SEARCH COMPLETED -    594 TO ITERATE

100.0% PROCESSED     594 ITERATIONS                          6 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        10418 TO    13342
PROJECTED ANSWERS:               6 TO      266

L2            6 SEA SSS SAM L1

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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED -  12211 TO ITERATE

100.0% PROCESSED   12211 ITERATIONS                         75 ANSWERS
SEARCH TIME: 00.00.01

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FILE LAST UPDATED: 30 Sep 2003  (20030930/ED)

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 substance identification.


=> s l3
L4           21 L3

=> s l4 and pd < january 1998
      18793762 PD < JANUARY 1998
                 (PD<19980100)
L5           16 L4 AND PD < JANUARY 1998

=> s l4 and guarna, a?/au
            104 GUARNA, A?/AU
L6            6 L4 AND GUARNA, A?/AU

=> s l5 not l6
L7           14 L5 NOT L6

=> s l6 not l5
L8            4 L6 NOT L5

=> d l5, ibib abs fhistr, 1-16
'FHISTR' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
```

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IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, IPC, and NCL

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):end

=> d his

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     FILE 'REGISTRY' ENTERED AT 15:43:30 ON 01 OCT 2003
L1             STRUCTURE UPLOADED
L2           6 S L1
L3          75 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 15:49:25 ON 01 OCT 2003
L4          21 S L3
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L5            16 S L4 AND PD <  JANUARY 1998
L6             6 S L4 AND GUARNA, A?/AU
L7            14 S L5 NOT L6
L8             4 S L6 NOT L5

=> d l5, ibib abs fhitstr, 1-16

L5   ANSWER 1 OF 16  HCAPLUS  COPYRIGHT 2003 ACS on STN
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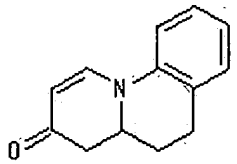
Full Text | Citing References

ACCESSION NUMBER: 1998:713257 HCAPLUS
DOCUMENT NUMBER: 130:52313
TITLE: Synthesis of benzo[c]quinolizin-3-ones: selective non-steroidal inhibitors of steroid 5α-reductase 1
AUTHOR(S): Guarna, Antonio; Occhiato, Ernesto G.; Scarpi, Dina; Tsai, Ruey; Danza, Giovanna; Comerci, Alessandra; Mancina, Rosa; Serio, Mario
CORPORATE SOURCE: Dipartimento di Chimica Organica "U. Schiff", Centro di Studio sulla Chimica e la Struttura dei Composti Eterociclici e lori Applicazioni, CNR, Univ. di Firenze, Florence, I-50121, Italy
SOURCE: Bioorganic & Medicinal Chemistry Letters (**1998**), 8(20), 2871-2876
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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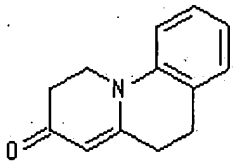
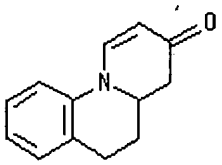


II

AB A short and efficient synthesis of novel benzo[c]quinolizin-3-ones I and II is described. The synthesis is based on the tandem Mannich-Michael cyclization between 2-(silyloxy)-1,3-butadienes and a N-t-Boc iminium ion. I and II are selective inhibitors of human steroid 5α-reductase isoenzyme 1, and thus have potential application as drugs for treatment of male pattern baldness and other DHT-dependent skin disorders.

IT **194979-80-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(benzo[c]quinolizin-3-ones as selective inhibitors of steroid 5α-reductase 1)
RN 194979-80-1 HCAPLUS
CN 3H-Benzo[c]quinolizin-3-one, 4,4a,5,6-tetrahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:542448 HCAPLUS
DOCUMENT NUMBER: 127:220585
TITLE: Benzo[c]quinolizine derivatives, their preparation and use as 5α-reductases inhibitors
INVENTOR(S): Guarna, Antonio; Serio, Mario
PATENT ASSIGNEE(S): Applied Research Systems ARS Holding N.V., Neth. Antilles; Guarna, Antonio; Serio, Mario
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 9729107	A1	19970814	WO 1997-EP552	19970207	<--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9717672	A1	19970828	AU 1997-17672	19970207	<--
AU 711886	B2	19991021			
EP 880520	A1	19981202	EP 1997-903230	19970207	
EP 880520	B1	20030416			
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EE 9800233	A	19981215	EE 1998-233	19970207	
EE 4058	B1	20030616			
CN 1210536	A	19990310	CN 1997-192097	19970207	
CN 1116296	B	20030730			
JP 2000504680	T2	20000418	JP 1997-528158	19970207	
AT 237614	E	20030515	AT 1997-903230	19970207	
EP 926148	A1	19990630	EP 1997-122733	19971223	
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NO 9803444	A	19980724	NO 1998-3444	19980724	
US 6303622	B1	20011016	US 1998-117583	19980729	
CA 2315055	AA	19990708	CA 1998-2315055	19981221	
WO 9933828	A1	19990708	WO 1998-EP8582	19981221	
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TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

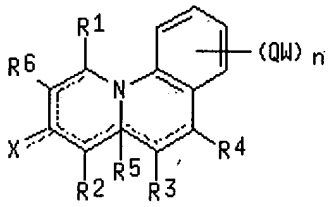
AU 9924194	A1	19990719	AU 1999-24194	19981221
AU 744105	B2	20020214		
BR 9813836	A	20001010	BR 1998-13836	19981221
EP 1066284	A1	20010110	EP 1998-966711	19981221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
EE 200000387	A	20011217	EE 2000-20000038	719981221
JP 2001527074	T2	20011225	JP 2000-526509	19981221
ZA 9811762	A	19990623	ZA 1998-11762	19981222
NO 2000003199	A	20000823	NO 2000-3199	20000620
US 2001044542	A1	20011122	US 2001-888952	20010625
US 6555549	B2	20030429		
US 2001047098	A1	20011129	US 2001-891088	20010625
US 6552034	B2	20030422		

PRIORITY APPLN. INFO.:

IT 1996-FI19	A	19960209
WO 1997-EP552	W	19970207
EP 1997-122733	A	19971223
US 1998-117583	A1	19980729
WO 1998-EP8582	W	19981221

OTHER SOURCE(S): MARPAT 127:220585

GI



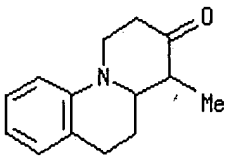
I

AB The benzo[c]quinolizine derivs. I (R1-R4, R6 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocycle, halo, amino azide, alkoxycarbonyl, etc.; R5 =H, alkyl, alkoxycarbonyl, cyano, aryl, heterocycle; X = O, acyl, alkoxycarbonyl, NO2, carbamoyl; Q = bond, alkyl, alkenyl, alkynyl, amino, etc., W = H, alkyl, alkenyl, alkynyl, aryl, aryloxy, amino, halo, etc.) were prepd. as 5α-reductases inhibitors (no data). Thus, N-(tert-butoxycarbonyl)-2-ethoxy-1,2,3,4-tetrahydroquinline was cyclized with 2-(trimethylsilyloxy)-1,3-butadiene to give 1,2,4,4a,5,6-hexahydro-(11H)-benzo[c]quinolizin-3-one.

IT **5569-24-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzo[c]quinolizine derivs. as 5α-reductases inhibitors)

RN 5569-24-4 HCAPLUS

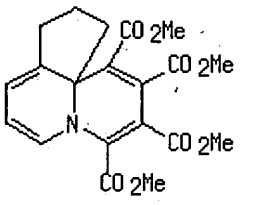
CN 3H-Benzo[c]quinolizin-3-one, 1,2,4,4a,5,6-hexahydro-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1985:595974 HCAPLUS
DOCUMENT NUMBER: 103:195974
TITLE: Addition reactions of heterocyclic compounds. Part 81. Products from dimethyl acetylenedicarboxylate with some cycloalkyl[b]pyridines
AUTHOR(S): Abbott, Patrick J.; Acheson, R. Morrin; Choi, Michael C. K.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, OX1 3QU, UK
SOURCE: Journal of Chemical Research, Synopses (**1985**), (6), 169
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:195974
GI



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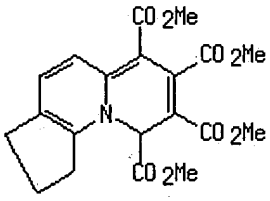
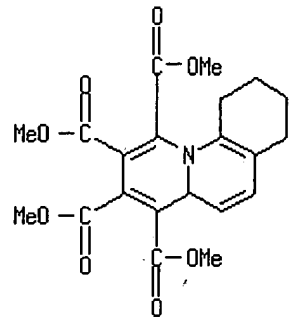


III

AB Treatment of cycloalkyl[b]pyridines with MeO2CC≡CCO2Me (I) gave tetra-Me 9aH-quinolizine-1,2,3,4-tetracarboxylates along with other quinolizines and oxoquinolizines. E.g., treatment of 6,7-dihydro-5H-cyclopenta[b]pyridine with I in DMF for 12 days gave tetracarboxylates II and III.

IT **99087-66-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 99087-66-8 HCAPLUS
CN 7H-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a,8,9,10-tetrahydro-, tetramethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1980:110806 HCAPLUS
DOCUMENT NUMBER: 92:110806
TITLE: Addition reactions of heterocyclic compounds. Part 69. Further studies of reactions between 2-alkylquinolines and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. Morrin; Procter, Garry
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, OX1 3QU, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1979**), (9), 2171-9
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
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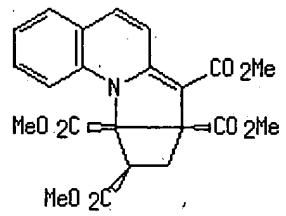


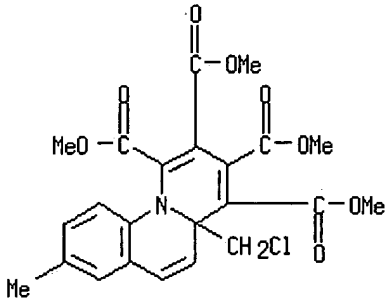
II

AB The reactions of MeO2CC≡CCO2Me (I) with Et quinoline-2-acetate, other quinolines with activated 2-Me groups, and 2-acetoxyquinoline were studied spectroscopically. Mechanistic schemes are proposed for the formation of cyclobutapyrroloquinoline II by the cycloaddn. reaction of 2-methylquinoline with I. Reactions of II, based on its previously reported azepine structure (A. et al., 1968), are reinterpreted using 13C NMR data.

IT **72813-97-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 72813-97-9 HCAPLUS

CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-(chloromethyl)-8-methyl-, tetramethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1979:491477 HCAPLUS
DOCUMENT NUMBER: 91:91477
TITLE: Addition reactions of heterocyclic compounds. Part 67. Products from 1-phenylbut-1-yn-3-one with various heterocycles, and from dimethyl acetylenedicarboxylate with some 2-substituted pyridines
AUTHOR(S): Acheson, R. Morrin; Wallis, John D.; Woollard, John
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1979**), (3), 584-90
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
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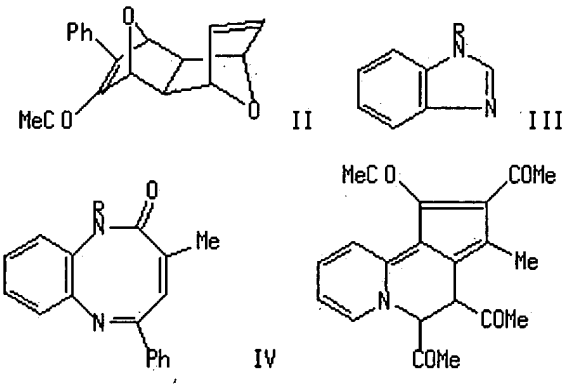
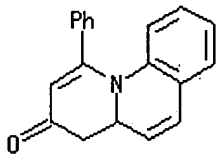


AB Treating PhC≡CCOMe (I) with 1-alkylpyrroles effected dimerization, whereas with furan, the adduct II was formed. With 3-methylpyridine and quinoline, I gave dihydroquinolizinones. Treating I with benzimidazole (III; R = H) gave mainly Z-III (R = CPh:CHCOMe) with some of the corresponding E-isomer whereas with III (R = Me, Et, CH2Ph), ring expansion to benzodiazocinones IV took place. Treating 1-(2-pyridyl)butan-2-one with MeO2CC≡CCO2Me gave quinolizine V, whereas other pyridines gave quinolizines, azepines, and indolizines.

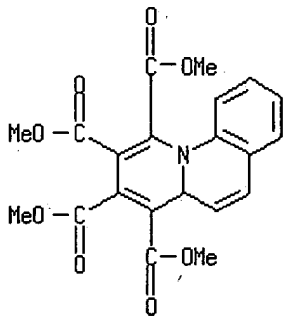
IT **71127-12-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 71127-12-3 HCAPLUS
CN 3H-Benzo[c]quinolizin-3-one, 4,4a-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1975:111924 HCAPLUS
DOCUMENT NUMBER: 82:111924
TITLE: Photoisomerization of benzo[c]quinolizines. Isolation of the first 2H-quinolizines derivative
AUTHOR(S): Plunkett, A. Owen
CORPORATE SOURCE: Dep. Chem., Portsmouth Polytech., Portsmouth, UK
SOURCE: Tetrahedron Letters (**1974**), (48), 4181-2
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Irradn. of tetra-Me 4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylate (I) in C6H6 gave the 3H-benzo[c]quinolizine II, the 1H tautomer of I, a benzo[c]indolizine, and a red dimer.
IT **26593-23-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(isomerization of, photochem.)
RN 26593-23-7 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1973:491951 HCAPLUS
DOCUMENT NUMBER: 79:91951
TITLE: Addition reactions of heterocyclic compounds. LII. Adducts from substituted 2-methylquinolines and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. Morrin; Nisbet, Donald F.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxf., Oxford, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1973**), (13), 1338-46
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

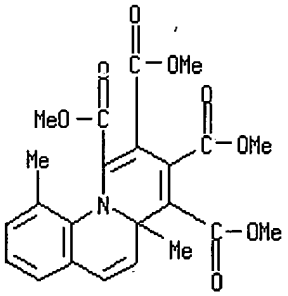
AB Mono-, di-. and trimethylquinolines with MeO2CC≡CCO2Me gave dark red adducts of two types, thought to be geometric isomers. E.g. 2-methylquinoline with MeO2CC≡CCO2Me gave a mixt. contg. hexa-Me 6,7,7a,8-tetrahydrobenzo[f]cyclopenta[a]quinolizine-6,7,7a,8,9,-10-hexacarboxylate (I) and an isomer. Other products from these reactions included benzo[c]quinolizine-, azepino [1,2-a]quinoline-, and 2-propenylquinolinecarboxylates. 2,8-Dimethyl- and 2,4,6,8-tetramethylquinoline also gave 2-[tris(methoxycarbonyl)phenyl]quinolines.

IT **49616-77-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 49616-77-5 HCAPLUS

CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a,10-dimethyl-, tetramethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:540662 HCAPLUS

DOCUMENT NUMBER: 75:140662

TITLE: Addition reactions of heterocyclic compounds. XLV. New azepines from substituted 2-methylquinolines and dialkyl acetylenedicarboxylates

AUTHOR(S): Acheson, R. M.; Nisbet, D. F.

CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (**1971**), (19), 3291-6
CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

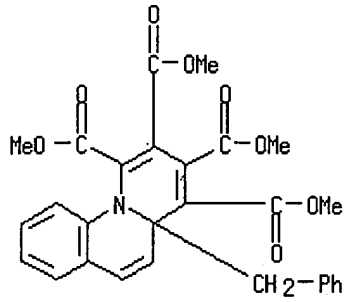
AB 3- and 4-Substituted 2-methylquinolines (e.g. 2,4-dimethylquinoline) reacted with MeO2CC≡CCO2Me to give tetra-Me 10,11-dihydroazepino-[1,2-a]quinoline-7,8,9,10-tetracarboxylates (e.g. I) and tetra-Me 4a-methyl-4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylates (e.g. II). 2-Benzylquinoline reacted similarly, but 2-ethyl-and 2,3-dimethylquinoline gave mixts. of the azepinoquinoline-7,8,9,10- and -7,8,9,11-tetracarboxylates.

IT **33898-14-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 33898-14-5 HCAPLUS

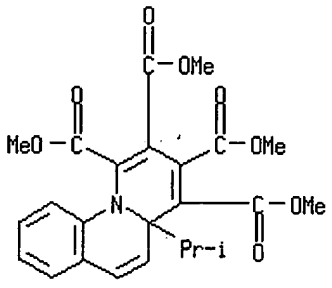
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-benzyl-, tetramethyl ester (8CI) (CA INDEX NAME)



L5 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:540657 HCAPLUS
DOCUMENT NUMBER: 75:140657
TITLE: Addition reactions of heterocyclic compounds. XLIV. Synthesis and photoisomerism of some quinolizine esters
AUTHOR(S): Acheson, R. M.; Stubbs, J. K.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1971**), (19), 3285-91
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB D labeling showed that the thermal rearrangement of tetra-Me 4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylate into the 1H-isomer is an intramol. process whereas the photochem. conversion involves D exchange with MeOH as solvent. MeO2CC≡CCO2Me reacted with 2-isopropyl- and 2-styrylquinoline, 2,3-dihydro-1H-cyclopenta[b]quinoline, and 1,2,3,4-tetrahydroacridine to give tetra-Me 4a-isopropyl- and 4a-styryl-4aH-benzo[c]quinolizine-1,2,3,4-tetracarboxylates, tetra-Me 6,7-dihydro-5H-benzo[c]cyclopenta[j]quinolizine-1,2,3,4-tetracarboxylate (I), and tetra-Me 5,6,7,8-tetrahydrodibenzo[cj]quinolizine-1,2,3,4-tetracarboxylate (II), resp. Irradn. of these quinolizines and other quinolizines with bridgehead H atoms or alkyl groups caused migration of the bridgehead group to C-1 in sterically favorable cases, sometimes with the formation of pyrroloazepines.
IT 33922-40-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and photochem. rearrangement of)
RN 33922-40-6 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-isopropyl-, tetramethyl ester (8CI) (CA INDEX NAME)



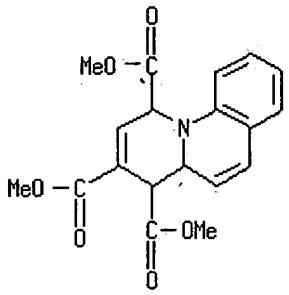
L5 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1971:529616 HCAPLUS
DOCUMENT NUMBER: 75:129616
TITLE: Addition reactions of heterocyclic compounds. XLVI. Reactions of acetylenic esters with pyridines in the presence of proton donors, and with alkyl 3-(2-pyridyl)-trans-acrylates
AUTHOR(S): Acheson, R. M.; Woollard, J. McK.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1971**), (19), 3296-305
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 3,5-Dimethylpyridine and HC≡CCO2Me gave Me 1,2-dihydro-1-[trans-2-(methoxycarbonyl)vinyl]-3,5-dimethyl-2-pyridinepropiolate. Pyridine and its 3-Me and 3,5-di-Me derivs. reacted with HC≡CCO2Me-MeOH to give Me 1,2-dihydro-2-methoxy-1-pyridineacrylates, and with HC≡CCO2-Me-H2O to give Me 1-pyridineacrylates contg. a (methoxycarbonylvinyloxy)(methoxycarbonyl)vinyl side chain. Reaction of 3,5-dimethylpyridine with HC≡CCO2Me-PhOH gave a 1:19 mixt. of Me cis and trans-phenoxyacrylates. Et 3-(2-pyridyl)-trans-acrylate with acetylenic mono- and diesters gave 4H-quinolizines via a spiro intermediate, with apparent migration of an ester group.

IT **33802-96-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 33802-96-9 HCAPLUS
CN 1H-Benzo[c]quinolizine-1,3,4-tricarboxylic acid, 4,4a-dihydro-, trimethyl ester (8CI) (CA INDEX NAME)



L5 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1970:3340 HCAPLUS
DOCUMENT NUMBER: 72:3340
TITLE: Addition reactions of heterocyclic compounds. XLI. Photolysis of some quinolizine esters
AUTHOR(S): Acheson, Richard M.; Stubbs, J. K.
CORPORATE SOURCE: Dep. Biochem., Oxford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (**1969**), (17), 2316-19
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

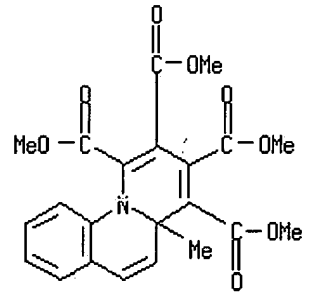
AB The irradn. of some tetramethyl 9aH-quinolizine-1,2,3,4-tetracarboxylates gave low yields of pyrrolo[1,2-a]azepines (e.g. I); similar 4aH-benzo[c]quinolizines gave corresponding 1H-isomers and other compds. The NMR and mass spectra and mode of formation of the products are discussed.

IT **17260-83-2**

RL: RCT (Reactant); RACT (Reactant or reagent)
(photolysis of)

RN 17260-83-2 HCAPLUS

CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-methyl-, tetramethyl ester (7CI, 8CI) (CA INDEX NAME)



L5 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1968:68849 HCAPLUS

DOCUMENT NUMBER: 68:68849

TITLE: Addition reactions of heterocyclic compounds. XXX. Acetylenedicarboxylic esters with benzopyridines possessing activated methyl groups

AUTHOR(S): Acheson, Richard M.; Gagan, J. M. F.; Harrison, Derek R.

CORPORATE SOURCE: Dep. Biochem., Oxford, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (**1968**), (4), 362-78
CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

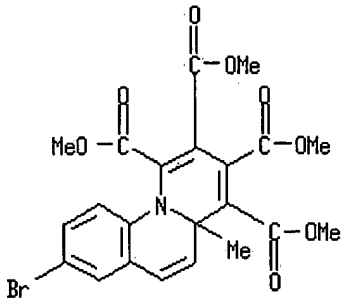
AB Dimethyl and diethyl acetylenedicarboxylate, with 2-methylquinoline and some derivs., 1-methylisoquinoline, and 6-methylphenanthridine, give dihydroazepines with the migration of an ester group; benzoquinolizines, such as I, and other products are also formed. The N.M.R. spectra of the ethoxycarbonyldihydroazepines and some derivs. were fully analyzed. Hydrogenation, protonation, bromination, hydrolysis, and oxidn. of the azepines were investigated, and a scheme for their formation is proposed. The N.M.R. spectra for some benzoquinolizines are tabulated. 36 references.

IT **17247-10-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 17247-10-8 HCAPLUS

CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 8-bromo-4a-methyl-, tetramethyl ester (8CI) (CA INDEX NAME)



L5 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1966:35773 HCAPLUS
DOCUMENT NUMBER: 64:35773
ORIGINAL REFERENCE NO.: 64:6613b-h,6614a-h,6615a-h,6616a-b
TITLE: Synthesis of 9-azasteroids. II. Synthesis of β-cyano- and β-carbethoxy-3-and 4-oxo-1,2,3,4,5,6-hexahydrobanzo[c]quinolizines
AUTHOR(S): Jones, G.; Wood, J.
CORPORATE SOURCE: Univ. Keele, UK
SOURCE: Tetrahedron (**1965**), 21(10), 2961-71
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 64, 2048c. The synthesis of 3- and 4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizines with reactive ester or nitrile groups situated so as to allow addn. of a 4th ring (ring D of the final 9-azasteroid) was reported. The previously prepd. oxo ester (I, 12.4 g.) in 100 ml. dry PhMe treated portionwise with 1.3 g. NaH (50% paraffin mull) and the mixt. refluxed 1 hr. with stirring, the cooled soln. treated with 9.63 g. MeI in 25 ml. PhMe and the stirred soln. slowly heated in 1 hr. to boiling, refluxed 2 hrs. and the cooled mixt. dild. with 100 ml. dry Et2O, the filtered soln. evapd. and the brown oil (5.5 g.) sepd. on Al2O3 gave the alkylation product (II), b0.0002 125-30°, and its stereoisomer, b0.0002 140-5°. Alternative routes to the non-enolizable oxo ester (III) were investigated. EtOCH2CH2OH (300 g.) and 350 g. PBr3 mixed slowly below 80° and stirred 1 hr. poured into 500 ml. ice-H2O and the washed and dried bromide distd. at 50 mm. gave 285 g. EtOCH2CH2Br. K (40.4 g.) in 800 ml. dry Me3COH stirred 30 min. at 50° with 150 g. MeCH(CO2Et)2 and the mixt. refluxed 2 hrs. with stirring with 178 g. EtOCH2CH2Br, the solvent evapd. and the residue treated at 0° with 400 ml. ice-H2O and Et2O yielded 161 g. EtOCH2CH2CMe(CO2Et)2 (IV), b10 130-2°. The ester (26 g.) in 200 ml. abs. alc. satd. with HBr and kept 16 hrs., refluxed 2 hrs. and evapd. in vacuo, the residual mixt. poured into 50 ml. ice-H2O and the aq. layer basified with NaHCO3, extd. with Et2O and the dried ext. distd. yielded 74% substantially pure BrCH2CH2CMe(CO2Et)2 (V), b11 138-40°. IV (102 g.) in 600 ml. 33% HBr boiled 6 hrs. with periodic distn. of EtBr, and removal of HBr in vacuo, HBr distd. in vacuo and the distillate neutralized, satd. with NaCl and extd. with Et2O, the extd. lactone and the carboxylactone distn. residue combined, heated 1 hr. at 200° and distd. yielded 73% 2-methyl-4-butyrolactone (VI),b11 81°. VI (32 g.) in 80 ml. abs. alc. satd. with HBr at 0° and the mixt. kept 24 hrs. at 20°, resatd. with HBr and kept 12 hrs. before pouring onto 120 g. ice, the ester layer and Et2O washings of the aq. layer combined and the washed and dried soln. distd. gave material, b1.0

45-50°, contaminated with 10% VI. Further washing with H2O and distn. gave pure BrCH2CH2CHMeCO2Et (VII), b1.0 47°. VII (49 g.), 24 g. Et 1,2,3,4-tetrahydroquinaldinate, 32.3 g. anhyd. K2CO3, and 1 g. KI heated 6 hrs. at 160-70° with vigorous stirring and the cooled mixt. treated with cold H2O and CHCl3, the CHCl3 layer dried and distd. at 10 mm. to give 12.1 g. VI and the pressure reduced gave 8.9 g. fraction, b0.18 104-40°. Further distn. at 0.0006 mm. yielded 61% material, b0.0006 140-60°, redistd. to give pure Et N-(3-ethoxycarbonylbutyl)-1,2,3,4-tetrahydroquinaldinate (VIII), b0.0006 154-6°. VIII (11.5 g.), 21.5 g. V, and 10.6 g. anhyd. K2CO3 heated 7 hrs. at 160° with stirring and the product fractionally distd. gave mainly VIII, 2-ethoxycarbonyl-2-methyl-4-butyrolactone, and 8% required Et N-[3,3-bis(ethoxycarbonyl)butyl]-1,2,3,4-tetrahydroquinaldinate, b0.0006 150°. VIII (8.65 g.) in 60 ml. dry xylene added in 30 min. to KOBu-tert (from 1.09 g. K) in 50 ml. refluxing xylene with distn. of evolved BuOH, the cooled mixt. dild. with 300 ml. dry Et2O and the hygroscopic K salt (6.0 g.) converted to the unstable base gave the acyloin (IX), HCl salt, m. 96-7°. Since the major difficulty in alkylating the cyclic ester I appeared to be competitive N-alkylation the basicity of the N was deactivated by nitration in the para-position using N2O4 in CCl4 according to Schaarschmidt et al. (CA 19, 2036). Et N-(3-ethoxycarbonylpropyl)-1,2,3,4-tetrahydroquinaldinate (X, R = H, 5.0 g.) in 50 ml. dry CCl4 at -5° stirred vigorously with 1.6 g. powd. CaCO3 with addn. of 1.45 g. N2O4 in 20 ml. CCl4 and the mixt. stirred 3 hrs. at -5°, warmed slowly and filtered at 20°, washed with 100 ml. cold 3N HCl, satd. aq. NaHCO3, and H2O and the dried soln. evapd. yielded 83% brown oil. A sample distd. in a bulb tube gave X (R = NO2) (XI), b0.001 200-10°. I (4.77 g.) in 100 ml. CCl4 at -5° stirred 30 min. with addn. of 1.69 g. N2O4 in 40 ml. ice-cold CCl4 and the mixt. stirred 3 hrs., the soln. decanted at 20° and the decantation and CCl4 washings evapd. yielded 24% solid. Recrystn. of a sample gave the nitro oxoester (XII, R = H) (XIII), m. 126-9°. XIII (1.35 g.) in 30 ml. PhMe added slowly to 50 ml. refluxing PhMe contg. of KOBu-tert (from 0.18 K) and the mixt. refluxed 30 min., the cooled mixt. treated with 1.2 g. MeI in 20 ml. PhMe and the mixt. slowly heated and refluxed 3 hrs., cooled and the filtered soln. evapd. gave an unstable gum, corresponding to the expected methylated compd. XII (R = Me). XI (0.66 g.) in 100 ml. alc. hydrogenated over 0.1 g. prereduced PtO2 with adsorption of 3 molar equivs. H gave 0.61 g. brown oil, distd. to give the amino diester X (R = NH2), b0.0003 185-95°. The previously synthesized cyano ester (XIV, 8.16 g.) in 75 ml. xylene added in 1 hr. with stirring to 2.25 g. NaOEt in 75 ml. boiling xylene with slow distn., the stirred mixt. refluxed 1 hr. and distd. to vapor temp. 138°, the ice-cold suspension dild. with 100 ml. each of Et2O and H2O and the org. layer extd. with 100 ml. N aq. NaOH, the combined aq. layers adjusted with 5N HCl at 0° to pH 6 and extd. with CHCl3, the residue on evapn. (6.41 g. brown gum) purified by regeneration from the HCl salt and a sample distd. gave 3-cyano-4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine, b0.003 180°; HCl salt, m. 163° (decompn.). Nitration of the cyano ketone gave an extremely insol. brown solid which has not been characterized. The major difficulty in synthesis of 4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine derivs. appeared to be inherent instability of systems which are formally analogous to 3-oxo-N-phenylpiperidine and synthesis of the probably more stable 3-oxo derivs. was undertaken. Attempts to synthesize the potentially useful intermediate tricyclic oxo ester (XV, R = H) (XVI) were undertaken. The initial approach was that of cyclization of the diester, Et 1-(2-ethoxycarbonylethyl)-1,2,3,4-tetrahydro-2-quinolyl acetate (XVII). Abs. alc. (300 ml.) and 4 ml. H2O contg. 29.4 g. 2-quinolylacetonitrile (from 2-chloromethylquinoline HCl salt) satd. with HCl at 60° and

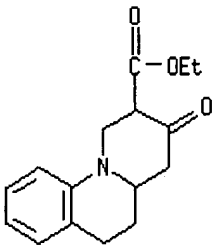
boiled 3 hrs., the chilled mixt. filtered and the residue on evapn. in vacuo treated with ice-cold satd. aq. NaHCO3, extd. with Et2O and the product distd. yielded 76% Et 2-quinolylacetate, b0.5 136-7°. The acetate (36.65 g.) in 250 ml. AcOH hydrogenated over prereduced PtO2 with 2 moles H and the residue on evapn. treated with aq. NaHCO3 and Et2O, the Et2O layer dried and distd. yielded 92% Et 1,2,3,4-tetrahydro-2-quinolylacetate (XVIII), b0.6 130-8°; 1-benzoyl deriv., m. 96.5-7.0° (ligroine). XVIII (10 g.), 16.42 g. BrCH2CH2CO2Et (b2.5 44°), 9.5 g. finely ground K2CO3, and 0.38 g. KI heated 4 hrs. at 140° under a short air condenser and the cooled mixt. treated with H2O and Et2O, the Et2O layer and washings dried and evapd., the residual oil distd. at 12 mm. to give 4 g. BrCH2-CH2CO2Et and at 0.003 mm. gave 1.7 g. XVIII and 63% yield of XVII, b0.003 145-60°, redistd. to give a sample, b0.003 161°. XVII (12.0 g.) cyclized with EtONa (from 0.95 g. Na in 200 ml. xylene) and the chilled (0°) mixt. treated with 100 ml. H2O, the aq. layer adjusted to pH 6.5 and dild. with Et2O, the org. layer and subsequent Et2O exts. combined and evapd. gave 93% viscous orange oil, purified by regeneration from the HCl salt to give the alternative quinazoline (XIX, R = H) (XX); HCl salt, m. 130° (Me2CO-Et2O-HCl). The cyclized Na salt suspension from 6.0 g. XVII treated at 0° with 3.06 g. MeI in 25 ml. xylene, stirred 1 hr. at 20 and 8 hrs. at 60°, the cooled mixt. filtered and the filtrate and Et2O washings evapd., the light-brown oily mixt. (3.86 g.) chromatographed on neutral Al2O3 from ligroine-C6H6 gave XV (R = Me) (XXI), b0.0004 130-4°, and the major isomer (XIX, R = Me) (XXII), b4 150-5°. The light brown oil (2 g., prepd. as above) boiled 6 hrs. in 5N HCl and evapd., the residue treated with aq. NaHCO3 and the free base extd. with Et2O yielded 73% 2-methyl-3-oxo-1,2,3,4,-5,6-hexahydrobenzo[c]quinolizine (XXIII), b0.003 130-40°. After equilibration with alc. EtONa the redistd. XXIII showed only the doublet at 0.99 ppm. Further confirmation that XXIII was a mixt. of epimers and not of structural isomers was obtained by hydrolyzing and decarboxylating 0.223 g. of the pure major isomer XXII to give 88% XXIII, practically identical with that obtained from the mixt. of oxo esters XXII. The equilibrated ketone XXIII heated 15 min. at 100° with a molar equiv. of 2,4-(O2N)2C6H3NHNH2 in abs. alc./HBr and the cooled mixt. filtered, the salt taken up in CHCl3 and shaken vigorously with aq. Na2CO3 and H2O, dried and evapd. gave XXIII dinitrophenylhydrazone, m. 195-8°. To identify the ketone and hence to deduce the direction of the Dieckmann cyclization in the di-ester XVII, attempts were made to synthesize XXIII or its isomer 4-methyl-3-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine (XXIV), but attempts to alkylate XVIII with Me2CBrCO2Et were unsuccessful in the production of XXIII. Quinaldyllithium (from 252 g. quinaldine) in Et2O added to 268 g. MeI under gentle reflux and the mixt. refluxed 1 hr., kept 16 hrs. at 20° and treated with 1300 ml. 5N HCl, the acid layer sepd. and the Et2O layer extd. with acid, the combined acid layers basified with NH4OH (d. 0.880) and the bases extd. with Et2O gave 47 g. quinaldine and 57% yield of 2-ethylquinoline, b14 134-5°. A filtered soln. of PhLi (from 90 g. PhBr) added slowly with stirring to 75 g. 2-ethylquinoline in 100 ml. Et2O and the mixt. refluxed 1 hr., the filtered 2-ethylquinolyllithium added in 1 hr. with stirring to 34 g. Et2CO3 in 100 ml. Et2O and the mixt. boiled 3 hrs., the cooled soln. treated with 500 ml. ice-cold 5N HCl, the acid layer and acid exts. neutralized with NH4OH and extd. with Et2O, evapd. and the residue distd. gave 29 g. 2-ethylquinoline b0.05 60-85°, and 15% yield of Et 2-(2-quinolyl)propionate (XXV), b0.05 116°; picrate, m. 137-40° (alc.). XXV (15.8 g.) in 150 ml. AcOH hydrogenated over 0.3 g. prereduced PtO2 with 2 moles H, the filtered soln. evapd. and the residue shaken with aq. NaHCO3 and Et2O, the Et2O ext. dried and distd.

gave 85% tetrahydro ester (XXVI) (R = H, R' = CHMeCO2Et) (XXVII), b0.7 134-8°. XXVII (13.9 g.), 21.5 g. BrCH2CH2CO2Et, 12.4 g. K2CO3, and 0.5 g. KI vigorously stirred 6 hrs. at 150° and the cooled product worked up as for XVII gave mainly 8.18 g. XXVII, b0.002 90-120°, and a 73% yield of the diester XXVI (R = CH2CH2CO2Et, R' = CHMeCO2Et) (XXVIII), b0.002 148-54°. XXVIII (6.48 g.) in 50 ml. xylene added slowly to KOCMe3 (from 0.836 g. K) in 75 ml. boiling xylene with slow distn. continued 1 hr., the cooled mixt. treated with 100 ml. ice-H2O and acidified to pH 6, extd. with Et2O and the residue on evapn. gave 2-ethoxycarbonyl-4-methyl-3-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizine (XXIX); HCl salt, melting to a thick glass at 50-5°, mobile at 85-90°. XXIX (2.5 g.) boiled 5 hrs. in 50 ml. 5N HCl and the residue on evapn. at 14 mm. treated with satd. aq. NaHCO3 and Et2O, the Et2O ext. dried and distd. gave a ketone, recrystn. from ligroine gave colorless rods, m. 96-7°; 2,4-dinitrophenylhydrazone, m. 153-5°. XXIII and XXIV differed markedly in ir absorption between 1450 and 700 cm.-1 and had retention times of 16.0 and 14.8 min. at 150°. Accordingly the C-methylation decarboxylation product was XXIII, the methylated keto ester XXII and the Dieckmann cyclization of XVII gave the oxo ester XX, unsuitable for further use in a 9-azasteroid synthesis. In view of the high yield obtained in cyclization of the cyano ester XIV it was decided finally to prep. and cyclize the isomeric cyano ester XXVI (R = CH2CH2CO2Et, R' = CH2CN) (XXX). XVIII (18 g.) in 500 ml. dry MeOH satd. with NH3 at 0° and autoclaved 40 hrs. at 100°, the soln. evapd. and the gum triturated with ligroine yielded 85% XXVI (R = H R' = CH2CONH2) (XXXI), m. 98-103°, recrystd. from C5H6 to give a sample m. 103-4°; N-Bz deriv., m. 198-201° (alc.). XXXI (12.5 g.) and 5.93 g. NaCl in 60 ml. ClCH2CH2Cl stirred 15 min. with addn. of 8.93 g. POCl3 in 10 ml. ClCH2CH2Cl, the mixt. warmed and boiled with stirring 12 hrs., the cooled mixt. treated with 8.0 g. NaOH in MeOH and shaken out twice with cold brine, the org. layer dried and distd. yielded 72% XXVI (R = H, R' = CH2CN) (XXXII), b0.06 124-7°; N-Bz deriv., m. 130° (alc.). XXXII (5.0 g.), 10.47 g. BrCH2CH2CO2Et, 6.02 g. K2CO3, and 0.24 g. KI heated 6 hrs. at 140° with stirring, the crude product isolated as for XVII and heated 8 hrs. at 145° with 10.5 g. BrCH2CH2CO2Et and 6 g. K2CO3, worked up again as for XVII to give 1.6 g. XXXII, b0.0006 110-35° and 80% yield of XXX, b0.0006 156-62°, m. 66° (ligroine). XXX (2.96 g.) in 50 ml. xylene added in 1 hr. with stirring to EtONa (from 0.275 g. Na) in 60 ml. boiling xylene and the boiling mixt. stirred 1 hr., worked up as for the cyano ketone from XIV to give 82% light yellow solid, m. 132-8°, recrystd. from alc. to colorless rhombs of the cyano ketone (XXXIII), m. 135.0-7.5°; HCl salt, m. 133-41° (Me2CO); phenylhydrazone, m. 166-7° (alc.). Since the yields are good throughout the synthesis the intermediate required for elaboration of ring D is available in quantity.

IT **5100-62-9**, 1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-3-oxo-, ethyl ester, hydrochloride
(prepn. of)

RN 5100-62-9 HCAPLUS

CN 1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-3-oxo-, ethyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)

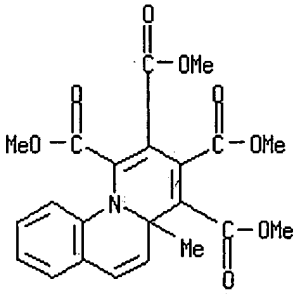


HCl

L5 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1963:3230 HCAPLUS
DOCUMENT NUMBER: 58:3230
ORIGINAL REFERENCE NO.: 58:504f
TITLE: The reaction of dimethyl acetylenedicarboxylate with quinaldine
AUTHOR(S): Crabtree, A.; Jackman, L. M.; Johnson, A. W.
CORPORATE SOURCE: Univ. Nottingham, UK
SOURCE: Journal of the Chemical Society, Abstracts (**1962**) 4417-20
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The main product from the reaction of dimethyl acetylenedicarboxylate and quinaldine is formulated as a tricyclic ylide (I) comprising a quinolinium ring with a fused seven-membered cyclic carbanion. The reactions and structure of the tetrabromo addn. product of I are discussed. The other product from the initial quinaldine reaction contains an angular methyl group and is a neutral quinolizine (II) which shows no tendency to rearrange.
IT **17260-83-2**, 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-methyl-, tetramethyl ester
(prepn. of)
RN 17260-83-2 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-methyl-, tetramethyl ester (7CI, 8CI) (CA INDEX NAME)



L5 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1962:403936 HCAPLUS
DOCUMENT NUMBER: 57:3936

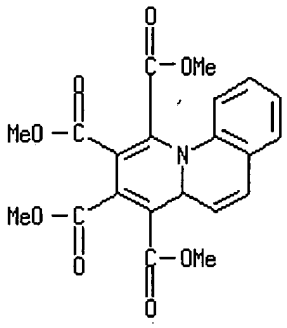
ORIGINAL REFERENCE NO.: 57:779a-g
TITLE: Addition reactions of heterocyclic compounds. IX. Benzoquinolizines from isoquinoline and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. M.; Hole, F.
CORPORATE SOURCE: Univ. Oxford, UK
SOURCE: Journal of the Chemical Society, Abstracts (**1962**) 748-52
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 55, 11391g; Diels and Harms, CA 30, 82234. From freshly distd. isoquinoline (I) and MeO2CC:CO2Me (II) was prepd. as described by D. and H. 77% D. and H's. "1st labile I adduct" (ascribed a different structure by D. and H.), m. 167°; this was now formulated as tetra-Me 11bH-benzo[a] quinolizine1,2,3,4-tetracarboxylate (III). When I was not freshly distd., only about 5% tri-Me benzo[g]indolizine-1,2,3-tricarboxylate (IV) was obtained. I (1 g.) in 5 ml. MeOH mixed with 2 ml. II in 3 ml. MeOH at room temp., kept 2 days, the ppt. collected, and chromatographed on Al2O3 gave IV, m. 154-5° (MeOH). I (8 ml.) in 10 ml. MeOH cooled to -32°, added dropwise to 11 ml. II in 30 ml. MeOH cooled to -32°, the mixt. allowed to rise to 0°, and kept 2 days at 0° gave 2.5 g. IV, identical (m.p., mixed m.p., and infrared absorption spectrum) with IV obtained above. III (1 g.) in 15 ml. AcOH and 5 ml. concd. H2SO4 kept 24 hrs. at 0°, treated with excess solid Na2CO3, and dild. with H2O gave tetra-Me 4H-benzo[a]quinolizine1,2,3,4-tetracarboxylate (V), m. 229-31° (AcOH); this compd. was given a different structure by D. and H. III (0.5 g.) in 5 ml. AcOH contg. 0.5 ml. 60% aq. HClO4 treated with 0.19 g. Br in 1.9 ml. AcOH and kept 16 hrs. gave 1,2,3,4-tetramethoxycarbonylbenzo[a]quinolizium (VI) perchlorate, m. 212° (decompn.) (AcOH). V (0.1 g.) in 5 ml. 1:1 aq.-MeOH treated with 2 g. Br, the mixt. refluxed 5 min., and concd. in vacuo gave VI perbromide, m. 140° (decompn.) (aq. MeOH). III (4 g.) in 30 ml. 1:1 aq.-MeOH treated rapidly with 2 g. Br, refluxed 1 min., and cooled gave 2.2 g. tetra-Me 6,7-dihydro-6-oxo-11bH-benzo[a]quinolizine-1,2,3,4-tetracarboxylate (VII), m. 207° (MeOH). III (4 g.) in 30 ml. 1:1 aq.-MeOH treated with 6 g. Br, refluxed 1 min., and cooled gave 1.7 g. tetra-Me 6 - (o - methoxycarbonylphenyl)pyridine - 2,3,4,5 - tetracarboxylate (VIII), m. 149-50° (MeOH), λ (MeOH) 2800 A. (ε 5800). VII (0.5 g.) in 10 ml. 1:1 aq. MeOH refluxed with 2 g. Br and evapd. in vacuo gave VIII, m.p. and mixed m.p. 149-50° (MeOH). III (1 g.) in 25 ml. MeOH contg. Raney Ni hydrogenated 14 hrs. at 4 atm., filtered, the filtrate concd. in vacuo, the residue shaken with 20 ml. cold MeOH, and the insol. product crystd. from MeOH gave tetra-Me x,x,6,7-tetrahydro-11 bH-benzo[a]quinolizine-1,2,3,4-tetracarboxylate (IX), m. 217°; evapn. of the MeOH ext. gave an isomeric tetrahydro compd., m. 124-6°. V (0.2 g.) in 25 ml. AcOH contg. PtO2 hydrogenated 14 hrs. at 4 atm. gave IX, m. 217°. Tetra-Me 6,7-dihydro11bH-benzo[a]quinolizine-1,2,3,4-tetracarboxylate (X) (0.2 g.) in 20 ml. MeOH contg. Raney Ni hydrogenated 2 hrs. gave IX, m. 217°. III (0.5 g.) in 25 ml. MeOH contg. 5% Pd-C hydrogenated at 4 atm. gave X, m. 179-80° (MeOH). The ultraviolet and infrared absorption spectra data of the adducts, some derivs., and related compds. were tabulated.

IT **26593-23-7**, 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester
(spectrum of)

RN 26593-23-7 HCAPLUS

CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



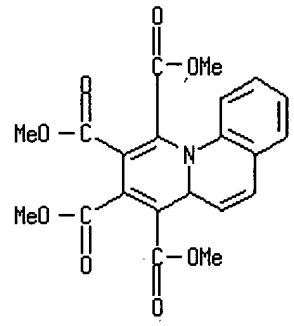
L5 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1961:13423 HCAPLUS
DOCUMENT NUMBER: 55:13423
ORIGINAL REFERENCE NO.: 55:2648g-i,2649a
TITLE: The adducts from quinoline and dimethyl acetylenedicarboxylate
AUTHOR(S): Acheson, R. M.; Earl, N. J.; Higham, P.; Richards, R. E.; Taylor, G. A.; Vernon, J. M.
CORPORATE SOURCE: Univ. Oxford, UK
SOURCE: Proc. Chem. Soc. (**1960**) 281-2
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB Quinoline and (MeO2CC≡)2 through a Diels-Alder reaction gave 2 1:2 adducts. The labile adduct (I) isomerized to the stable adduct (II) on heating or treatment with acids. Structures I and II were assigned to these adducts on the basis of similar compds. obtained in the pyridine series (CA 54, 18521a). I was nonbasic in HClO4-HOAc. Its structure was shown by nuclear magnetic resonance (n.m.r.) studies (Van Tamelen, et al., CA 54, 7704b). II did not react with Me2SO4 in MeNO2 at 100° and was monobasic to HClO4 in AcOH. It was a little less basic than tetra-Me 4H-quinolizine-1,2,3,4-tetracarboxylate (the stable pyridine adduct), as approx. 35% HClO4 in MeOH (instead of 8%) was required before the long-wavelength absorption band of the adduct completely disappeared. Diln. with water reversed the change. The hypsochromic shift of the long-wavelength absorption band by approx. 980 A. and other changes in the spectrum observed on acidification were of the magnitude expected for the conversion of the base into the cation.

IT **26593-23-7**, 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester
(prepn. of)
RN 26593-23-7 HCAPLUS
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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L2               6 S L1
L3              75 S L1 FULL

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L5              16 S L4 AND PD <  JANUARY 1998
L6               6 S L4 AND GUARNA, A?/AU
L7              14 S L5 NOT L6
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L9            5 L3

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L9   ANSWER 1 OF 5  CAOLD  COPYRIGHT 2003 ACS on STN
AN   CA64:6613c  CAOLD
TI   synthesis of 9-azasteroids - (II) synthesis of β-cyano- and
     β-carbethoxy-3- and 4-oxo-1,2,3,4,5,6-hexahydrobenzo[c]quinolizines
AU   Jones, Gurnos; Wood, J.
IT    539-74-2    592-55-2   1679-47-6   2213-09-4   5100-50-5   5100-51-6
     5100-52-7   5100-53-8   5100-54-9   5100-55-0   5100-56-1   5100-57-2
     5100-58-3   5100-59-4   5100-61-8   5100-62-9   5100-63-0
     5100-64-1   5100-65-2   5100-66-3   5100-67-4   5100-68-5   5100-69-6
     5100-70-9   5100-71-0   5100-72-1   5100-73-2   5100-74-3   5100-75-4
     5100-76-5   5100-77-6   5100-78-7   5161-93-3   5161-95-5   5161-98-8
     5161-99-9   5569-24-4   5688-31-3   6166-32-1  14283-09-1

L9   ANSWER 2 OF 5  CAOLD  COPYRIGHT 2003 ACS on STN
AN   CA64:6613b  CAOLD
TI   synthesis and reactions of 1-carbamoyl- 1 1-oxoindeno[1,2-c]isoquinoline
AU   Stowell, James K.
IT   5161-91-1   5161-92-2   5580-65-4

L9   ANSWER 3 OF 5  CAOLD  COPYRIGHT 2003 ACS on STN
AN   CA58:504e  CAOLD
TI   reaction of dimethyl acetylenedicarboxylate with quinaldine
AU   Crabtree, A.; Jackman, L. M.; Johnson, A. W.
IT  17260-83-2 100266-52-2 101358-50-3 107118-15-0

L9   ANSWER 4 OF 5  CAOLD  COPYRIGHT 2003 ACS on STN
AN   CA57:779g  CAOLD
TI   synthesis of 9, 11, 12, 13, 13a, 14-hexahydro-2,3,6-
     trimethoxydibenzo[f,h]pyrrolo[1,2-b]isoquinoline
AU   Govindachari, Tuticorin R.; Ragade, I. S.; Viswanathan, N.
IT    909-41-1   1971-34-2   4176-23-2   4234-95-1  24892-72-6  26593-23-7
     30963-47-4  33922-39-3  59222-31-0  87101-69-7  93431-38-0  93809-59-7
     94005-32-0  94165-06-7  97434-62-3 100088-44-6 100233-74-7 100233-81-6
     100266-53-3 101984-30-9 105767-03-1 107160-62-3

L9   ANSWER 5 OF 5  CAOLD  COPYRIGHT 2003 ACS on STN
AN   CA55:2648g  CAOLD
TI   adducts from quinoline and dimethyl acetylenedicarboxylate
AU   Acheson, Roy M.; Earl, N. J.; Higham, P.; Richards, R. E.; Taylor, G. A.;
     Vernon, J. M.
IT    762-42-5  26593-23-7  33922-39-3 132753-02-7


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RN   5100-62-9  REGISTRY
CN   1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-3-oxo-,
     ethyl ester, hydrochloride (7CI, 8CI)  (CA INDEX NAME)
MF   C16 H19 N O3 . Cl H
LC   STN Files:   CA, CAOLD, CAPLUS
CRN  (5161-92-2)
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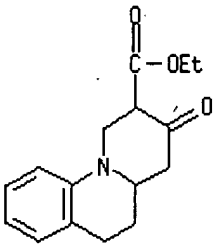

HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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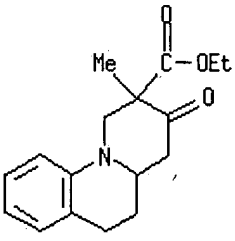
ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 5100-63-0 REGISTRY
CN 1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-2-methyl-3-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H21 N O3
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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=> **fil reg; d acc 5100-64-1; fil CAOLD**

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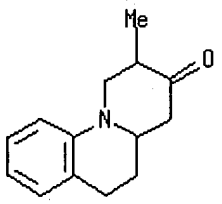
ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 5100-64-1 REGISTRY
CN 3H-Benzo[c]quinolizin-3-one, 1,2,4,4a,5,6-hexahydro-2-methyl- (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H17 N O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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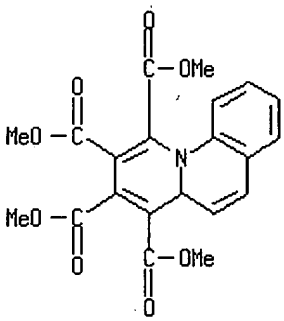
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 15:52:07 ON 01 OCT 2003

=> **fil reg; d acc 26593-23-7; fil CAOLD**

FILE 'REGISTRY' ENTERED AT 15:52:12 ON 01 OCT 2003

ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 26593-23-7 REGISTRY
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H19 N O8
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



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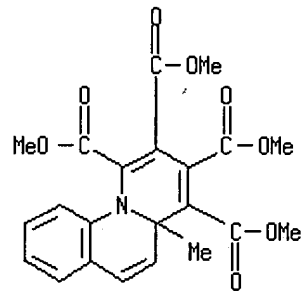
=> **fil reg; d acc 17260-83-2; fil CAOLD**

FILE 'REGISTRY' ENTERED AT 15:52:26 ON 01 OCT 2003

ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 17260-83-2 REGISTRY
CN 4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, 4a-methyl-, tetramethyl ester (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H21 N O8
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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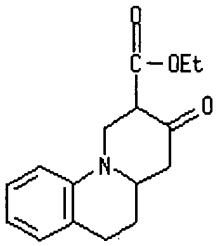
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 15:52:26 ON 01 OCT 2003

=> **fil reg; d acc 5161-92-2; fil CAOLD**

FILE 'REGISTRY' ENTERED AT 15:52:37 ON 01 OCT 2003

ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 5161-92-2 REGISTRY
CN 1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-3-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H19 N O3
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT
(*File contains numerically searchable property data)



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1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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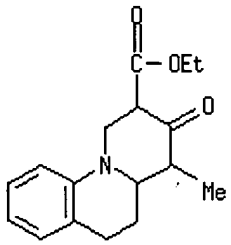
ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 5100-71-0 REGISTRY
CN 1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-methyl-3-oxo-, ethyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)
MF C17 H21 N O3 . Cl H
LC STN Files: CA, CAOLD, CAPLUS
CRN (5100-70-9)



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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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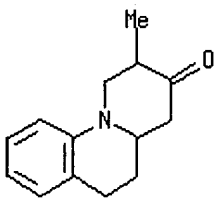
=> fil reg; d acc 5100-64-1; fil CAOLD

FILE 'REGISTRY' ENTERED AT 15:53:04 ON 01 OCT 2003

ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 5100-64-1 REGISTRY
CN 3H-Benzo[c]quinolizin-3-one, 1,2,4,4a,5,6-hexahydro-2-methyl- (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H17 N O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



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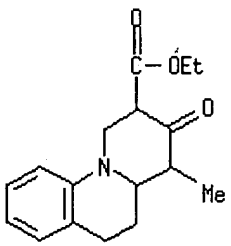
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 15:53:05 ON 01 OCT 2003

=> **fil reg; d acc 5100-70-9; fil CAOLD**

FILE 'REGISTRY' ENTERED AT 15:53:17 ON 01 OCT 2003

ANSWER 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 5100-70-9 REGISTRY
CN 1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-methyl-3-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H21 N O3
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

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              1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
              1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)


FILE 'CAOLD' ENTERED AT 15:53:17 ON 01 OCT 2003

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.40     257.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -10.42

STN INTERNATIONAL LOGOFF AT 15:53:29 ON 01 OCT 2003
```

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	SEP 09	CA/CAplus records now contain indexing from 1907 to the present
NEWS 4	Jul 15	Data from 1960-1976 added to RDISCLOSURE
NEWS 5	Jul 21	Identification of STN records implemented
NEWS 6	Jul 21	Polymer class term count added to REGISTRY
NEWS 7	Jul 22	INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available
NEWS 8	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS 9	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 10	AUG 15	PATDPAFULL: one FREE connect hour, per account, in September 2003
NEWS 11	AUG 15	PCTGEN: one FREE connect hour, per account, in September 2003
NEWS 12	AUG 15	RDISCLOSURE: one FREE connect hour, per account, in September 2003
NEWS 13	AUG 15	TEMA: one FREE connect hour, per account, in September 2003
NEWS 14	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS 15	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS 16	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Righ Truncation
NEWS 17	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS 18	SEP 22	DIPPR file reloaded
NEWS 19	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS 20	SEP 29	DISSABS now available on STN

NEWS EXPRESS	OCTOBER 01 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:00:27 ON 01 OCT 2003

=> **file reg**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:00:33 ON 01 OCT 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2
DICTIONARY FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

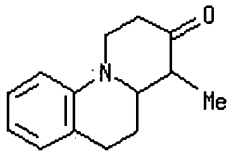
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

```
=> e 5569-24-4/cn
E1            1     5568: PN: WO9514772 SEQID: 5563 CLAIMED SEQUENCE/CN
E2            1     5569 PN: WO0118542 TABLE: 3A-1 CLAIMED DNA/CN
E3            0 --> 5569-24-4/CN
E4            1     5569: PN: EP1281758 SEQID: 5600 UNCLAIMED DNA/CN
E5            1     5569: PN: US20010051335 SEQID: 5569 CLAIMED DNA/CN
E6            1     5569: PN: US20020137160 SEQID: 5569 CLAIMED DNA/CN
E7            1     5569: PN: US6617156 SEQID: 5569 CLAIMED PROTEIN/CN
E8            1     5569: PN: WO0078341 PAGE: 71 UNCLAIMED SEQUENCE/CN
E9            1     5569: PN: WO0122920 SEQID: 6645 CLAIMED SEQUENCE/CN
E10           1     5569: PN: WO0142792 TABLE: 8A-1 CLAIMED DNA/CN
E11           6     5569: PN: WO0146697 TABLE: 21 CLAIMED DNA/CN
E12           1     5569: PN: WO0147944 SEQID: 5521 CLAIMED SEQUENCE/CN

=> e 5569-24-4/rn
E1            1     5569-19-7/RN
E2            1     5569-22-2/RN
E3            1 --> 5569-24-4/RN
E4            1     5569-25-5/RN
E5            1     5569-26-6/RN
E6            1     5569-27-7/RN
E7            1     5569-28-8/RN
E8            1     5569-29-9/RN
E9            1     5569-30-2/RN
E10           1     5569-31-3/RN
E11           1     5569-32-4/RN
E12           1     5569-34-6/RN

=> s e3
L1            1 5569-24-4/RN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS on STN
RN   5569-24-4  REGISTRY
CN   3H-Benzo[c]quinolizin-3-one, 1,2,4,4a,5,6-hexahydro-4-methyl- (7CI, 8CI,
     9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C14 H17 N O
```

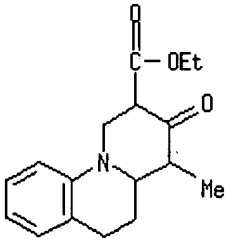
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

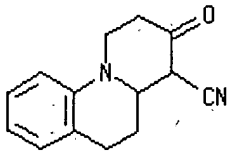
```
=> e 5100-70-9/rn
E1            1      5100-68-5/RN
E2            1      5100-69-6/RN
E3            1 --> 5100-70-9/RN
E4            1      5100-71-0/RN
E5            1      5100-72-1/RN
E6            1      5100-73-2/RN
E7            1      5100-74-3/RN
E8            1      5100-75-4/RN
E9            1      5100-76-5/RN
E10           1      5100-77-6/RN
E11           1      5100-78-7/RN
E12           1      5100-80-1/RN

=> s e3
L2            1 5100-70-9/RN

=> d l2

L2   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS on STN
RN   5100-70-9  REGISTRY
CN   1H-Benzo[c]quinolizine-2-carboxylic acid, 2,3,4,4a,5,6-hexahydro-4-methyl-
     3-oxo-, ethyl ester (7CI, 8CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C17 H21 N O3
CI   COM
LC   STN Files:   BEILSTEIN*, CA, CAOLD, CAPLUS
         (*File contains numerically searchable property data)
```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

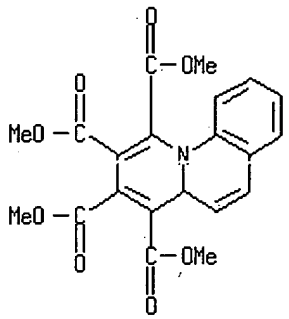
1 REFERENCES IN FILE CA (1907 TO DATE)

```
                1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)


=> e 5100-76-5/rn
E1              1     5100-74-3/RN
E2              1     5100-75-4/RN
E3              1 --> 5100-76-5/RN
E4              1     5100-77-6/RN
E5              1     5100-78-7/RN
E6              1     5100-80-1/RN
E7              1     5100-81-2/RN
E8              1     5100-82-3/RN
E9              1     5100-83-4/RN
E10             1     5100-84-5/RN
E11             1     5100-85-6/RN
E12             1     5100-86-7/RN

=> s e3
L3              1 5100-76-5/RN

=> d l3

L3   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS on STN
RN   5100-76-5  REGISTRY
CN   1H-Benzo[c]quinolizine-4-carbonitrile, 2,3,4,4a,5,6-hexahydro-3-oxo-,
     hydrochloride (7CI, 8CI)  (CA INDEX NAME)
MF   C14 H14 N2 O . Cl H
LC   STN Files:   CA, CAOLD, CAPLUS
CRN  (5100-77-6)
```



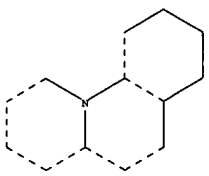

```
      # HCl
                1 REFERENCES IN FILE CA (1907 TO DATE)
                1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)


=> e 26593-23-7/rn
E1              1     26593-17-9/RN
E2              1     26593-20-4/RN
E3              1 --> 26593-23-7/RN
E4              1     26593-26-0/RN
E5              1     26593-27-1/RN
E6              1     26593-29-3/RN
E7              1     26593-33-9/RN
E8              1     26593-34-0/RN
E9              1     26593-35-1/RN
E10             1     26593-36-2/RN
E11             1     26593-37-3/RN
E12             1     26593-38-4/RN
```

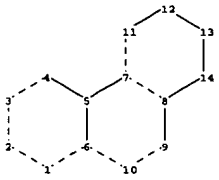
```
=> s e3
L4            1 26593-23-7/RN

=> d l4

L4   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS on STN
RN   26593-23-7  REGISTRY
CN   4aH-Benzo[c]quinolizine-1,2,3,4-tetracarboxylic acid, tetramethyl ester
     (6CI, 7CI, 8CI, 9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C21 H19 N O8
LC   STN Files:   BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER
         (*File contains numerically searchable property data)
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               6 REFERENCES IN FILE CA (1907 TO DATE)
               6 REFERENCES IN FILE CAPLUS (1907 TO DATE)
               2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)


=> log y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               7.52       7.73

STN INTERNATIONAL LOGOFF AT 16:01:49 ON 01 OCT 2003
```

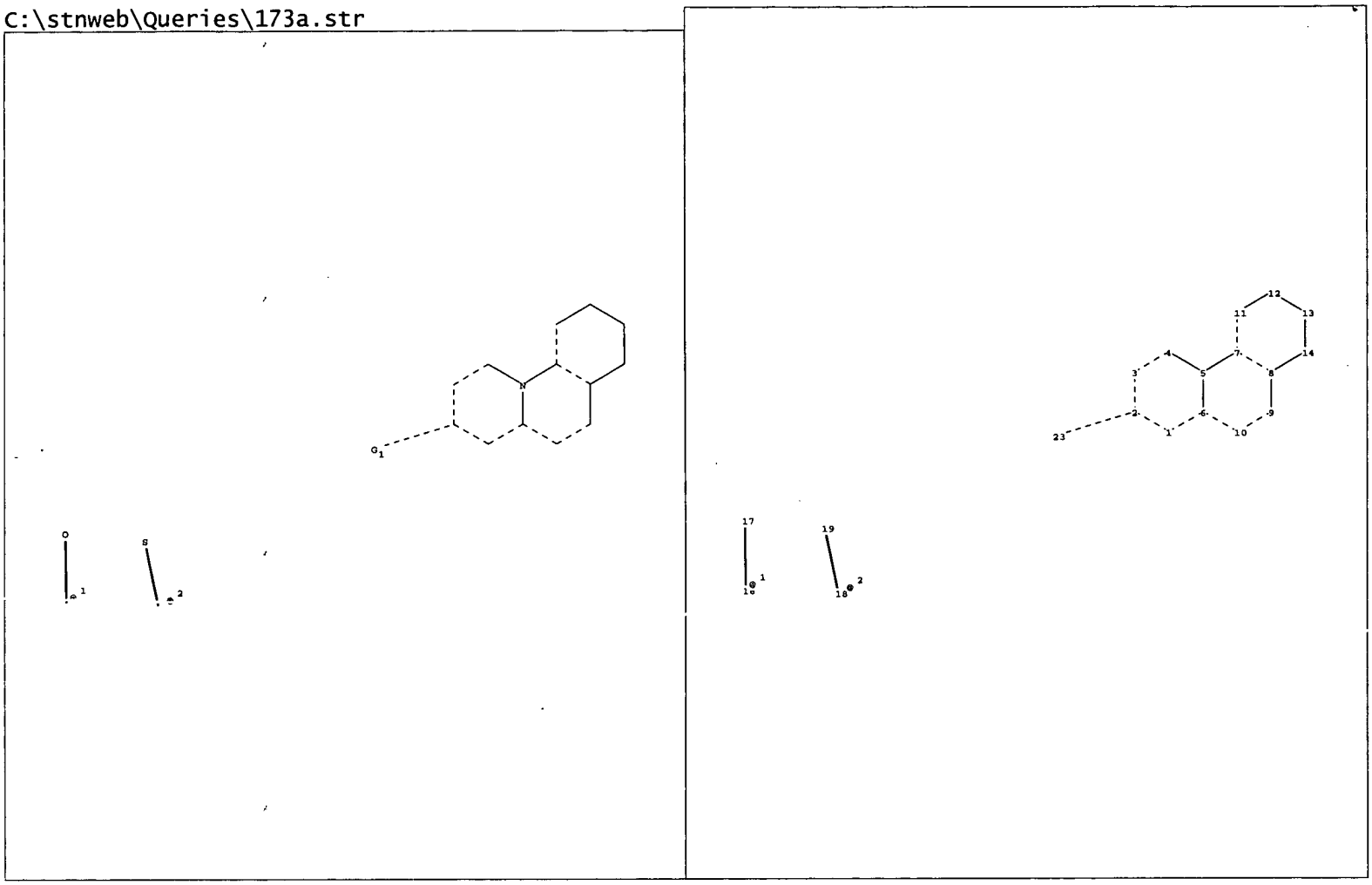
C:\stnweb\Queries\173.str





```
ring nodes :
    1  2  3  4  5  6  7  8  9  10  11  12  13  14
ring bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  7-11  8-9  8-14  9-10  11-12  12-13  13-14
exact/norm bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  7-11  8-9  8-14  9-10  11-12  12-13  13-14
isolated ring systems :
    containing 1 :

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom  11:Atom
    12:Atom  13:Atom  14:Atom
```

C:\stnweb\Queries\173a.str



chain nodes :
16 17 18 19 23
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14
chain bonds :
2-23 16-17 18-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14
exact/norm bonds :
1-2 1-6 2-3 2-23 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13
13-14 16-17 18-19
isolated ring systems :
containing 1 :

G1:O,S,NO2,[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 23:CLASS